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Modified Gravity in the Primordial Universe

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Especialização em Astrofísica e Cosmologia

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2024

Agradecimentos

Todo o percurso que fiz até agora não foi feito inteiramente sozinho. Como tal, não poderia deixar de lado um conjunto de agradecimentos escritos pelo coração.

Antes de mais e quaisquer outros agradecimentos, o primeiro agradecimento que dedico é um pessoal e é dado é ao meu Lorde e Salvador, Jesus Cristo.

Esta tese envolveu um conjunto amplo de pessoas e o seu existir é muito graças aos meus dois orientadores Dr. José Pedro Mimoso e Dr. Francisco S.N. Lobo que foram pessoas fulcrais para mim. Quero então agradecer profundamente ao Dr. José Pedro Mimoso e ao Dr. Francisco S.N. Lobo por todo o apoio, ensinamentos e por me guiarem para o começo da minha vida como investigador. Quero agradecer especialmente ao Professor Mimoso pelas incontáveis, incansavéis e marcantes reuniões que tivemos no seu gabinete, as tardes bem passadas, e ao Professor Lobo pelos concelhos, criticas que me guiaram sempre de forma a ser um melhor investigador e pela valiosa direção que me apontou no mundo da investigação ao qual estou imensamente agradecido. Queria também agradecer aos professores Nelson Nunes, António Silva e Ana Arriaga da Faculdade de Ciências pelas aulas fascinantes que deram e pela empenhada pedagogia que me permitiu desfrutar dos estudos académicos.

Desde de muito criança, por volta dos cinco anos, que desenvolvi uma "panca" por física, como se diz na gíria popular. Neste meu bichinho pela física, a minha Mãe desempenhou um papel fundamental e singular tendo-me sempre apoiado com tudo e um pouco mais. Na verdade, se há pessoa que me apoia em tudo e por tudo é a minha Mãe, uma pessoa que admiro muito e me inspira de forma totalmente sem paralelo, gostava de ser metade da pessoa que és Mãe. As coisas maior parte do tempo não foram fáceis mas tens a magia de conseguir resolver as coisas todas e se nunca senti o amargo da fome, frio e desamparo foi devido a ti Mãe. Quero deixar aqui um agradecimento profundo e com toda alma a ti Mãe, por todos os sacrifícios, lutas e amor. Aqui quero deixar também um agradecimento ao meu Pai. Por todos aqueles almoços alegres e cheios de vida, pelas boleias da estação para casa onde muito falamos, as "piratices" que só nós fazemos, todos os concelhos de pai que me deu principalmente na adolescência e todo o apoio que só um pai pode dar.

Dentro da física, o meu maior fascínio foi sempre a astrofísica e este fascínio foi alimentado em parte pelos conhecimentos sobre a área que a minha Mãe me passou e do entusiasmo que a Madrinha tem sobre esta área tão intrigante. Para além deste contributo queria agradecer à minha Madrinha por todo o apoio que me deu, a mim e à minha Mãe, especialmente quando era eu era bebé e criança. Infelizmente não segui uma área que permite dar o teu nome a um asteroide Madrinha, mas melhor que cosmologia não há! Quero também agradecer a quem cá já não está mas que no coração ficará para sempre e quem sempre terá a sua essência e humanidade única lembrada, obrigado Padrinho, por teres sido como foste e pela tua genuinidade.

Não podia faltar um agradecimento à malta amiga e especial. Em primeiro lugar quero agradecer à Carolina Pires por tudo o que aturou/atura de mim, por ser a namorada que é, por todo o apoio e amor que deu durante o escrever desta tese e no geral, apoio esse que foi fundamental, e por todos os momentos inesquecíveis - que seja assim para sempre. Em segundo lugar agradeço aos meus amigos do coração, a Catarina Matos e o Gonçalo Baião, que ao fim de 8 e 5 anos de me aturarem ainda continuam todos os dias a tornar a nossa interação sem igual. Obrigado Bióloga e Engenheiro de computação quântica, o Artesão adora-vos. Aproveita esta deixa para agradecer a mais dois amigos do coração que conheci na Faculdade de Ciências, o Hélder (o meu irmão perdido) e o Miguel (o meu colega da vida de bairro). Ao meu maninho Hélder agradeço pelas ideias elaboradas que debatíamos em conjunto, pelos momentos de apoio em todas as situações de stresse académico e pelos debates políticos no café do C8. Quero agradecer ao Miguel pela orientação inicial que deu no meu mestrado e pelos momentos de riso passados na FCUL, a cosmologia aguarda-nos. Para os melhores físicos futuros que já vi, um obrigado rapazes. Durante a licenciatura e mestrado conheci diversas pessoas que tornaram os estudos académicos mais dinâmicos e melhores. Portanto, quero agradecer ao João Galupa, o homem das noitadas em trabalho e convívio, ao Tomaz Zalez o meu "beto" favorito, ao Tiago Rodrigues, o melhor jogador de futebol, à Leonor Ferro, a minha companheira do café do C8 e irmã em Cristo, ao Tiago Gonçalves pelas vezes que o chateei com as minhas ideias e ao Pedro Gamito por ter ido a todas as minhas aulas de duvidas de Relatividade Geral e Cosmologia e pelos livros de física que me arranjou.

A todos os que foram mencionados aqui, aos que não foram mencionados mas que estão nas entrelinhas, e aos que cá já não estão, um obrigado profundo.

Resumo

De todas as épocas que o nosso Universo passou, a época Primordial é a fase mais intrigante e repleta de questões em aberto. Desde do próprio começo do Universo às previsões dos primeiros elementos leves que foram cruciais para o evoluir do Universo, a fase primordial do Universo tem um papel extremamente valioso na compreensão absoluta da evolução do nosso Universo.

O sucesso da nossa compreensão e descrição atual desta época é alcançado usando a descrição moderna da cosmologia que é construida com base na Relatividade Geral em conjunto com o modelo padrão de partículas. Contudo, apesar deste sucesso, diversos problemas existem que põem em questão se não é necessário alterar algum destes dois modelos. Problemas ao nível da descrição mais tardia do Universo, como a origem da expansão acelerada e a tensão da constante de Hubble, podem ser vistas como fortes indícios que é necessário uma nova física. Para apoiar ainda mais este ideia, problemas nas fases iniciais do Universo, como a origem teórica da inflação, a assimetria entre matéria e anti-matéria e a disparidade entre as observações do lítio primordial face ao previsto teoricamente, são também pontos bastante relevantes que apoiam a necessidade de nova física. Adicionalmente, o facto de o modelo padrão de partículas apontar para uma unificação das três interações fundamentais que descreve: interação eletromagnética, interação fraca e interação forte, a altas energias, pode ser também usado como um racional para argumentar que a gravidade a altas energias pode ter outra descrição e se essa nova descrição levaria a uma nova cosmologia e a uma nova física.

Começando pelo inicio do nosso Universo, o modelo cosmológico atual recorre à inflação, um período de expansão extremamente rápida que ocorreu nos instantes iniciais do Universo, proposta para resolver problemas do modelo padrão da cosmologia, como o problema do horizonte, da planura e da ausência de monopólos magnéticos. Durante essa fase, o Universo expandiu-se exponencialmente em uma fração de segundo, suavizando as irregularidades iniciais e levando à homogeneidade e isotropia observadas na radiação cósmica de fundo. Essa ideia, originalmente introduzida por Alan Guth, ganhou peso com a criação de modelos que envolvem um campo escalar chamado por vezes de inflatão, que seria responsável por este processo inflacionário. A inflação também fornece um mecanismo natural para a geração das flutuações de densidade que deram origem às estruturas cósmicas, ligando-se diretamente à teoria da perturbação cósmica. Contudo, a origem teórica da inflação ainda permanece sem uma resposta convincente estando muitas vezes associada a teorias de gravidade modificadas e a extensões ao modelo padrão da física de partículas

Adicionalmente, entre os desafios mais fundamentais e intrigantes do Universo Primordial, a assimetria observada entre matéria e anti-matéria destaca-se como um dos problemas centrais da cosmologia moderna. Esta questão, inicialmente vista como uma peculiaridade das condições iniciais do Universo, passou a ser encarada, a partir do trabalho seminal de Andrei Dmitrievich Sakharov, como um fenómeno que necessita de explicação dentro das próprias leis físicas que governam a evolução do Universo. Sakharov formulou três condições necessárias, hoje conhecidas como os "critérios de Sakharov", que qualquer modelo ou mecanismo capaz de explicar a assimetria matéria-antimatéria deve satisfazer. Estes

critérios estabelecem as bases para a criação de teorias sobre a geração de uma preferência pela matéria sobre a anti-matéria, sendo que tal processo é denominado de Bariogénese. Ao longo das últimas décadas, diversas abordagens teóricas foram propostas para explicar esta assimetria, onde a maioria delas são ancoradas na física de partículas e interações fundamentais, tratando a gravidade como um elemento secundário ou complementar. No entanto, uma proposta distinta surge ao colocar a gravidade no centro deste processo. Conhecida como Bariogénese Gravitacional, esta teoria difere das abordagens convencionais ao tratar a gravidade não apenas como um pano de fundo estático, mas como uma componente ativa e essencial na geração da assimetria. Este mecanismo sugere que a interação gravitacional desempenha um papel primordial na quebra de simetria entre matéria e anti-matéria, abrindo novas perspetivas para a compreensão dos processos que moldaram o Universo primordial.

Esta tese tem então como objetivo explorar o impacto de modificações à gravidade no contexto da bariogénese e inflação onde o foco principal será a assimetria entre matéria e anti-matéria.

Dito isto, começa-se por realizar uma introdução detalhada sobre as descrições que a gravidade já teve, como o modelo padrão de cosmologia foi criado, que problemas atualmente existem neste modelo onde foram expostos com detalhes os problemas (modernos e passados) associados à época primordial e finaliza-se este primeiro capitulo da tese com uma breve introdução a geometria diferencial e derivação da relatividade geral através do principio variacional.

No segundo capítulo, o modelo padrão cosmológico é apresentado com os detalhes necessários associado à sua aplicação ao Universo Primordial e adicionalmente é exposta uma descrição termodinâmica necessária para a descrição teórica da bariogénese.

O capitulo seguinte é dedicado a apresentar o contexto teórico associado à bariogénese. Os critérios de Sakharov são apresentados e explicados seguindo-se a exposição dos três mecanismos de bariogénese que foram trabalhados nesta tese: Bariogénese Eletro-fraca, Bariogénese através de Teorias da Grande Unificação e Bariogénese Gravitacional. As duas primeiras teorias são construidas sobre a estrutura teórica da física de partículas usando a gravidade como ferramenta de segunda ordem enquanto que o terceiro mecanismo, como já referido, usa a gravidade de forma mais fundamental. Os problemas associados a estes mecanismos são expostos com ênfase nos da Bariogénese Eletro-fraca uma vez que a gravidade pode ter um papel importante para os resolver. O problema em questão corresponde à capacidade deste mecanismo ter uma transição de fase de primeira ordem quando ocorre a transição eletro-fraca.

No capítulo 4, são introduzidas e detalhadas as duas teorias de gravidade modificada selecionadas para aplicação aos mecanismos discutidos no capítulo 3. Para os dois mecanismos de caráter menos dependente da gravidade, foi escolhida a teoria escalar-tensorial, enquanto para o terceiro mecanismo, mais centrado na gravidade, optou-se pela teoria $f(R,\mathcal{T}^2)$. São apresentadas as equações de campo associadas a ambas as teorias, bem como suas cosmologias e demais aspetos teóricos relevantes. Além disso, foi discutida a conexão entre os princípios teóricos da inflação cósmica e as teorias escalar-tensorial, destacando como estas influenciam o comportamento do Universo primordial.

No penúltimo capítulo, que precede o sumário e as conclusões, são expostos os resultados obtidos da aplicação dessas teorias de gravidade modificada aos diferentes mecanismos de bariogénese. No caso da teoria escalar-tensorial, observou-se que a modificação da taxa de expansão do Universo impacta significativamente os cenários de bariogénese. Com base no modelo cosmológico considerado, que se divide em três épocas, sendo a primeira dominada pelo campo escalar desta teoria, os resultados indicam compatibilidade com os principais constrangimentos impostos pela Bariogénese Eletro-fraca. Ademais, a aplicação da teoria escalar-tensorial aos mecanismos de Bariogénese através das Teorias da Grande Unificação também forneceu resultados preliminarmente positivos. Os resultados mais promissores, no

entanto, foram obtidos no contexto da Bariogénese Gravitacional onde diversos cenários de sucesso foram identificados, sendo que a teoria de $f(R,\mathcal{T}^2)$ se destacou ao apresentar o maior número de resultados positivos. Entre estes, o modelo que mais sobressaiu pode ser interpretado como uma versão ligeiramente modificada da Relatividade Geral, introduzindo um parâmetro adicional constante que ajusta as previsões cosmológicas padrão sugerindo um novo caminho para a compreensão da Bariogénese gravitacional.

Palavras chave: Gravidade Modificada, Universo Primordial, Cosmologia, Bariogénese, Inflação

Abstract

This thesis investigates fundamental questions related to the early Universe, particularly focusing on baryogenesis and cosmic inflation. While the current cosmological model, built on General Relativity and the Standard Model of particle physics, has been successful in describing many aspects of the Universe, unresolved issues, such as the matter-antimatter asymmetry, the origin of cosmic inflation, and the acceleration of the Universe's expansion, suggest the need for new physics. In this work, modifications to gravity, specifically scalar-tensor theories (STT) and the $f(R,\mathcal{T}^2)$ theory, are explored as potential solutions for the long last problem of the asymmetry between matter and anti-matter. To do such, the Electroweak baryogenesis mechanism and Baryogenesis thru Grand Unification Theories were explored using STT while Gravitational baryogenesis was explored using $f(R,\mathcal{T}^2)$. The relation between inflation and STT was also briefly exposed.

The results show that these alternative gravitational models can provide new insights into the mechanisms of baryogenesis, with the $f(R,\mathcal{T}^2)$ theory offering particularly promising outcomes for gravitational baryogenesis.

Keywords: Modified Gravity, Primordial Universe, Cosmology, Baryogenesis, Inflation

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Preface

The official research presented in this Master's thesis was conducted at the Instituto de Astrofísica e Ciências do Espaço (IA) and at the Departamento de Física da Faculdade de Ciências da Universidade de Lisboa, with support from the research grants UIDB/04434/2020 and UIDP/04434/2020. The research was supervised by Professors Francisco S. N. Lobo and José Pedro Mimoso from the Instituto de Astrofísica e Ciências do Espaço (IA) and the Departamento de Física da Faculdade de Ciências da Universidade de Lisboa (FCUL). The sections 5.1,5.2, in chapter 5, had the collaboration of João Ferraz, an ex-master student of Professor José Pedro Mimoso.

The content of this thesis is based on the following research papers published in refereed Journals:

- **Baryogenesis: a symmetry breaking in the primordial Universe revisited**
  David S. Pereira, João Ferraz, Francisco S. N. Lobo, José Pedro Mimoso
  Symmetry 2024, 16(1), 13 arXiv:2312.14080 [gr-qc]

- **Gravitational baryogenesis in energy-momentum squared gravity**
  David S. Pereira, Francisco S. N. Lobo, José Pedro Mimoso
  arXiv:2409.04623 [gr-qc]
  Under review: European Journal of Physics C

- **Thermodynamics of the Primordial Universe: A concise review**
  David S. Pereira, João Ferraz, Francisco S. N. Lobo, José Pedro Mimoso
  Under review: Entropy MDPI

Moreover, selected material of these papers was also presented at a national conference in talk format:

- David S. Pereira, "Matter and Anti-matter asymmetry: a possible solution from Modified Gravity", XXXIV Encontro Nacional de Astronomia e Astrofísica, September 12th, 2024, Guimarães.

During this thesis it was also produced the following article:

- **Extension of Buchdahl's Theorem on Reciprocal Solutions**
  David S. Pereira, José Pedro Mimoso Francisco S. N. Lobo
  Symmetry 2024, 16(7), 881 arXiv:2407.08320 [gr-qc]

Chapter 1

Introduction

1.1 So what is gravity?

1.1.1 Gravity from the ancient to Einstein, from Newton's apple to Cosmology

Gravity is, to date, probably the most enigmatic fundamental interaction and presents the greatest challenge when one tries to achieve a universal description. The path that led to our current understanding of gravity is full of contributions and built on advances that only giants could make such as Galileo, Newton and Einstein. Historically, gravity was the first interaction encountered by humanity and the first to be studied through experimental investigation. The famous Galileo Galilei introduced experimental tools like pendulums and incline planes to explore gravity at the terrestrial scale unavailing surprising properties of an interaction that we observe in our daily lives. In addition to this contribution, it was Galileo who established a relationship between references that are in movement, and Galileo's famous transformations. Newton brought the first mathematical description of gravity in a general thus cementing the beginning of the in-depth study of gravity. For a long time, Newton's description of gravity remained untouchable and reigned supreme being able to describe almost all the observations done by Kepler, classical physics and other phenomena. Despite the tremendous success of such a description, Newton's description of gravity was haunted by a single problem that would end Newton's absolute gravitational description in Physics.

The dethronement of Newton's gravity formalism started in the second half of the 19th century when observations of Mercury reported a strange behaviour in the precession of the perihelion of the planet that could not be explained by simply employing Newton's mechanics. Attempts to solve this problem without calling into question Newton's theory were the norm. The most famous effort came from Le Verrier, who speculated on the existence of a planet close to Mercury, never before observed, called Vulcan. However, there were no observations to support this theory and it quickly fell into oblivion. The answer would appear almost seventy years later at the hands of a young, courageous and curious German physicist. Seeking to extend his theory of special relativity [1], Albert Einstein developed the theory that today we call the best description of gravity: General Relativity (GR). Already dethroning Newton in his notion of absolute space and time, by introducing the idea of space and time being one entity and time being relative, Einstein boldly proposed a theory of gravity beyond expectations, a theory based on a geometric description that used differential geometry in a way that no one thought could be used to describe gravity in such a deep way. Finished and published in 1915, Einstein presented to the world the theory of General Relativity. This theory would be experimentally proven by the results observed for the precession of Merury's orbit, as well as other experimental outcomes like the Lense-Thirring gravitomagnetic precession (1918) and the gravitational deflection of light by the Sun, measured in 1919 during a Solar eclipse by Arthur Eddington, giving the final blow to Newton's theory of gravity declaring GR as the new best theory to describe gravity. Although such dethrone was received as a shock, GR had already started to receive a lot of attention and work developed since its theorization and soon, physicists started to see the "true power"of the generalization of special relativity. The first marvelous result came by the hands of a famous German physicist, that at the time of is contributions to GR was a German soldier fighting in the front lines of World War I. Karl Schwarzschild was the first physicist to find exact solutions for the Einstein field equations that described what we today call Black Holes. This result brought an intriguing description of the nature of gravity, space-time, describing perplexing phenomena such as the event horizon and, most important, the problem and notion of singularities in GR. Physics inside the core of a black-hole remains a problem without solution with GR being unable to answer the question: what happens inside the black-hole singularity. In 2019, the Event Horizon Telescope Collaboration present to the world the first strong evidence for the existence of this tremendous and mysterious objects [2]. Five years before, the LIGO (Laser Interferometer Gravitational-Wave Observatory) Scientific Collaboration and Virgo Collaboration announced the first direct detection of gravitational waves from the merging of two black-holes [3]. Both of this results sedimented General Relativity as a phenomenal theory of gravity.

Besides the ramifications of GR to astrophysics, GR presented the perfect (or maybe almost perfect) framework for dealing with the nature of the universe, its origins and its evolution. Starting with a paper published in 1917 by Albert Einstein [4], cosmology saw its birth. Initiating with a static description of the Universe, Einstein made the first kick to our comprehension of the Universe's evolution. Although this static description, motivated by the personal beliefs of Einstein, was received with some positivity its fate soon came when Edwin Hubble, using the Hooker Telescope, the world's largest telescope at the time, discovered that our Universe was not static, it was expanding [5]. This groundbreaking discovery lead to the developed of many cosmological descriptions of the Universe with different ideas, evolution's of the Universe and ends to it but only one prevailed as the best description, the Friedmann–Lemaître–Robertson–Walker description. This description refers to a category of universes that are homogeneous and isotropic (we will revisit this point later). Space-time divides into evenly curved space and cosmic time shared by all moving observers. This description is now recognized as the FLRW or Robertson-Walker metric. Equipped with such description, physicists unveiled the inner working of our Universe. The great dilemma of the beginning of the Universe saw a possible answer by the hands of a Belgian physicist who was also a Roman Catholic priest, Georges Lemaître. Having already given an important contribution to the conclusion that our Universe was not static but was in expansion, Lemaître inspired by the biblical teachings and description of the beginning of the Universe, Lemaître found that GR was able to describe a Universe that emerged from a single point, a "primordial atom". Such a bold claim received several critics, with the majority claiming that such a theory was religious-based and not scientific. Despite the criticism, the Big Bang theory, a name not given by Lemaître itself but by one of his critics, Fred Hoyle, prevailed as the favoured and best description of the beginning of our Universe standing out from the remaining competing theories when one of its most crucial prediction, the Cosmic Wave Background (CMB), was observed in 1964 at Bell Labs [6]. It can be said that this paved the way for modern cosmology, as from this point forward, the field saw a significant increase in contributions and studies with famous names such as Roger Penrose, Stephen Hawking, George F. R. Ellis and many others making important contributions. Another fundamental concept developed within the Big Bang theory is the cosmologic inflation [7], an epoch characterized by an exponential expansion that occurred in a extremely short interval of time. Even though the success of the Big Bang predictions and results, some shortcomings persisted such as the flatness problem, the Horizon problem and the Magnetic-monopole problem that can be all solved with inflation. The first problem stems from the observation that certain initial conditions of the universe seem to be finely tuned to very "special"values [8]. Small deviations from these values would have significant effects on the appearance of the universe at the present time. The Horizon problem is related to the reason connected to the Universe appearing homogeneous and isotropic at large scales. The last problem stems from the possible existence of Grand Unification theories (GUTs) [9], that unify the tree fundamental interactions of particle physics. At high temperatures, such as in the early universe, the electromagnetic force, strong, and weak nuclear forces are not fundamental forces but arise from spontaneous symmetry breaking of a single gauge theory and the problem comes from the prediction of magnetic monopoles from these theories that are a class of exotic particles never observed [10, 11]. Inflation can solve these three problems as a rapid expansion of the Universe is able to justify the horizon problem, to answer the fine tuning problem presented by the flatness problem and if magnetic monopoles were created a period of inflation occurring at a temperature below that at which magnetic monopoles can be produced, monopoles would be pushed apart as the universe expands, potentially reducing their observed density by several orders of magnitude. By the turn of the last century, the final ingredient to the modern cosmological description of the Universe was found, the expansion rate of the Universe was accelerating! Observations of the Type Ia supernovae confirmed that the Universe is currently experiencing an exponentially accelerated expansion, known as late-time cosmic acceleration [12, 13, 14, 15].

With all this, the current model of cosmology was developed, called the Standard Model of Cosmology (SMC), or ΛCDM [16] where Λ stands for the Cosmological constant [17] that is necessary to obtain an accelerated expansion and CDM denotes Cold Dark Matter. This model incorporates the several key ideas previously presented and as well observational results such as: the CMB, Baryonic Acoustic Oscillations [18, 19], the primordial power spectrum's and the capability to reproduced observed phenomena such as the large-scale structure in the distribution of galaxies, the observed abundances of hydrogen (including deuterium) and helium and the accelerating expansion of the universe observed in the light from distant galaxies and supernovae. In conjunction with the Standard Model of Particle Physics, a theoretical model that appeared much later than GR, these two models are our current best understanding of the Universe.

1.1.2 Cosmology with General Relativity describes well the late and the early Universe, right?

The remarkable achievements of GR make it a cornerstone of modern physics and the strong experimental evidence continues to support this theory as the best explanation for gravity. However, as the precision of measuring instruments has improved, and with the launched of new probes and telescopes that can test GR (such as the James-Webb Telescope, the Euclid Mission, and LISA, Laser Interferometer Space Antenna, in the future) and obtain more data for cosmology, tensions between GR predictions and observational data have emerged and increasingly indicate that GR may not be the ultimate description of gravity [16]. Many of these tensions are referred to as late-time tensions, meaning that they are related to the present time and not very far behind in the past of our Universe. From these tensions, the two that most stand out are the Hubble tension (see [20] for an in-depth review), where local measurements of the Hubble parameter are in tension with the value inferred from a ΛCDM that fit the CMB data, and the $\sigma 8$ tension where measurements of weak gravitational lensing at low redshifts indicate weaker matter clustering compared to what is expected from the standard ΛCDM cosmological model with parameters determined by CMB measurements[16]. Additionally, the standard model of cosmology has two major theoretical weaknesses. The major problem stems from the fact cosmological constant, which is equivalent to introducing a uniformly distributed form of energy, has no satisfactory theoretical description and observations rule out the best theoretical descriptions [21, 22, 23, 24, 25]. The second problem is related to GR in cosmology being incapable to justify the existence of dark matter, which is thought to constitute about 25% of the total matter/energy content present in the Universe [16, 26]. Even though dark matter is a theoretical prediction of particle physics that was not yet detected, its applications on the astrophysical domain as the most acceptable answer to the observed anomalous galactic rotation curves [27, 28] can be interpreted as a shortcoming of GR at the scales at question.

Although the problems associated with the late-time epoch of the Universe are well recognized, the primordial epoch also presents a significant number of unresolved questions and challenges. The primordial stage of the Universe is characterized by a unique theoretical framework, distinct from that of the late-time Universe, due to its extremely high energy scales. This epoch provides a natural laboratory for exploring high-energy physics. The Big Bang theory, which describes the origin of the Universe, posits an initial singularity, a singular point from which the Universe is thought to have emerged. However, this concept has faced criticism, as it could be interpreted as a limitation of General Relativity or even a flawed prediction of the Big Bang theory itself. Conceptually, the idea of an initial singularity is more intuitive, as it allows us to imagine a Universe beginning from a state of zero size with infinite temperature and energy density, where all fundamental interactions are unified within a still-unknown theoretical framework. Nonetheless, it is also possible that the Universe undergoes a cyclic cosmological evolution, in which it never actually contracts to a state of zero size. Subsequently, the Big Bang theory is intrinsically linked to the concept of inflation, as inflation addresses three significant cosmological problems that the Big Bang theory has. However, the true nature of inflation is not truly understood. From a theoretical point of view inflation is a simple mechanism but from a fundamental point of view inflation stands as a complex and profound unanswered question. Following this problem, in the time-line of the Universe evolution a fundamental problem also arises. The standard model of particle physics predicts that all particles burst into existence following same laws of physics with no reason for a unbalance in the production of particles or anti-particles. Therefore, total annihilation of particles and anti-particles would happen resulting in a Universe with only radiation. However, our own existence and astronomical observations [29, 30, 31] point out to the existence of an asymmetry between matter and anti-matter. Although the asymmetry observed is very small, of the order of 10^{-11}, the implications that this asymmetry brings to the evolution of the Universe are extremely important as it has impact in the formation of the first light elements. Andrei Dmitrievich Sakharov was one of the first physicists that try to solve this problem by introducing a "recipe" to generate and preserve the asymmetry [32]. This work laid the ground for the study of mechanisms able to generate this asymmetry that are denominated as baryogenesis mechanisms. Baryogenesis stands as the crucial theoretical field searching to solve this problem with mechanisms and phenomena that, in the majority of the cases, brings new physics typically in the form of extensions of the standard model of particle physics. Another problem connected to the primordial Universe is the lithium problem. The current model for the Big Bang Nuclesynthesis (BBN) [33], the process that formed the first light elements, hydrogen, deuterium, helium and lithium, in the Universe, and one of the only few probes of the very early Universe with direct experimental or observational consequence, when in combination with the data from the Wilkinson Microwave Anisotropy Probe (WMAP) cosmic baryon density show that the 7Li observations lie below the prediction [34]. A recent update on the numerical/computational side of the BBN calculation was achieve with the code *PRIMAT* [35, 36] but the lithium problem still persist. Diverse solutions have been proposed [37] ranging from observational problems, astrophysical processes, nuclear phenomena, modified statistics, exotic new physics in the early universe and changes to the cosmological description.

Additionally, in recent years, another (pseudo-)problem appeared due to the James Webb Space Telescope (JWST) [38] observations. The James Webb Space Telescope has identified exceptionally bright early galaxies, i.e, high-redshift galaxies with surprisingly high stellar masses [39, 40, 41], which suggests a potential conflict with the predictions of the ΛCDM cosmological model. Some solutions have been proposed both from an observational point of view [42] but the majority of the belief resides in modifications to ΛCDM such as non Gaussianities in primordial fluctuations [43], modified dark energy description [44], heavy primordial black-holes (PBHs) [45] or more exotic approaches as axion miniclusters [46]. The PBHs approach is particularly interesting as this objects can also be a viable candidate for DM [47, 48]. Another (pseudo-)problem is the anomalies of the CMB [16]. Additionally, with the future launch of LISA, the existence of Primordial Gravitational Waves, a phenomena that offers a unique glimpse into the early Universe and serve as the sole probe of the physics associated with the inflationary epoch will play a role on better understanding the primordial universe as many new physics predict this indirect observational and it will also serve to test and constraint the current cosmological model [49, 50, 51].

From a more fundamental and theoretical perspective, General Relativity also faces significant challenges, such as the presence of singularities. These singularities, typically associated with the centers of black holes, are regions of spacetime where both the curvature and the energy density of matter become infinite. The existence of such singularities suggests the need for a quantum theory of gravity. Moreover, when considering the very early stages of the Universe, it becomes essential to incorporate quantum corrections to General Relativity and idea explore by Alexei Alexandrovich Starobinsky [52] that eventually lead to his famous model for inflation.

1.1.3 If the standard model of cosmology has problems, what do we do?

With cosmology encountering a diverse array of challenges across two distinct epochs of the Universe, it raises the question of what strategies might effectively address these issues. While there are numerous potential approaches to tackling these problems, two major branches of research have emerged as particularly prominent. The first branch mainly focuses on modifications to the matter-energy sector, such as the introduction of unknown particles like axions, the introduction of neutrinos with unique behaviors like self-interaction or special interactions with dark matter, dark matter possessing particular properties such as self-interaction, and various models of dark energy. The latter includes numerous theoretical frameworks designed to construct a viable model, as discussed in the literature [20, 53, 54, 55]. These models encompass scalar fields, spinor fields, (non-)abelian vector theories, the cosmological constant, fluids with complex equations of state, and theories involving higher-dimensional spaces. From the late-time standpoint, the dark energy approach has is advantageous sides as it is able to obtain the late accelerated expansion of the Universe without much effort. Additionally, according to Lovelock's theorem [56, 57], the only possible second order Euler-Lagrange expression obtainable in a four-dimensional space from a scalar density of the form $\mathcal{L} \equiv \mathcal{L}(g_{\mu\nu})$ is $\mathcal{H}_{\mu\nu} = \sqrt{-g}(\lambda_1 G_{\mu\nu} + \lambda_2 g_{\mu\nu})$ where λ_1 and λ_2 are constants with one leading to Newton's gravitational constants, G, and the other to the cosmological constant, Λ, in the Einstein's field equations, therefore, the cosmological constant appears in a natural way. Furthermore, dark matter (for in-depth reviews see [26, 58, 59]) stands also as a strong theoretical contender to solve diverse problems in cosmology as it is a favorite among the others theoretical possibilities due to the belief that the standard model of particles has unknown sectors.

Alternatively, the previous problems and weaknesses related to GR can be used to argue that something new needs to appear, in other words, possibly a new theory of gravity. This logic leads to the second branch characterized by modifying the gravitational description and searching different theories of gravity that can tackle all the problems mentioned. Changes in the gravitational description lead to changes in the cosmological description and such modifications can answer the issues mentioned. Additionally, without a proper theory of quantum gravity, the search for this "holy grail"can also benefit from the study and exploration of modified theories of gravity. Modifications to gravity that go beyond GR are not a recent idea, as right after the publication of GR new theories of gravity were also proposed one of the most famous and early modified theories of gravity proposed was the Brans-Dicke scalar-tensor theory of gravity [60].

Numerous modified theories of gravity have been proposed; for a comprehensive reviews, see [61, 62, 63, 64] and the modern development of modified gravity theories can be traced back to the seminal work of Hans Adolf Buchdahl [65], in which he introduced a Lagrangian of the form $f(R)$, with R representing the Ricci scalar. By employing the variational principle, a theoretical framework that will become particularly important later, Buchdahl explored the cosmological implications of this theory.

1.1.4 Why modified gravity in the primordial Universe?

Given the energy scales characteristic of the primordial Universe, the primary focus of this thesis, it is reasonable to suggest that, like the three fundamental interactions described by the Standard Model of particle physics, which are unified under a Grand Unified Theory at high energy scales, gravity may also necessitate a different theoretical framework in such high energy regimes. Although this hypothesis appears straightforward, its implications and consequences are significantly more complex. This idea can be traced back to Paul Dirac, who in 1937 proposed the Large Number Hypothesis (LNH) [66]. Dirac's hypothesis suggests that the gravitational "constant"might not be constant at all but could instead vary over time. This concept eventually led to the development of the Brans-Dicke scalar-tensor theory of gravity—a theory in which the gravitational interaction is mediated by both a scalar field and the tensor field of general relativity. Dirac proposed that "any two of the very large dimensionless numbers occurring in nature are connected by a simple mathematical relation, in which the coefficients are of the order of magnitude of unity." For instance, the ratio of the electromagnetic to gravitational forces between a proton and an electron in a hydrogen atom, $\frac{e^2}{Gm_pm_e} \approx 10^{40}$, and the ratio of the age of the Universe to the atomic time unit, $\frac{m_e t_0}{e^2} \approx 10^{40}$, suggest a potential relationship between these large dimensionless quantities. Dirac believed that this apparent coincidence among various cosmological and atomic constants hinted at an as-yet-undiscovered theory that connects the quantum mechanical origins of the Universe to its cosmological parameters. Furthermore, during the very early epochs of the Universe, quantum gravitational processes may have played a crucial role in shaping its evolution [67, 68, 69], which further emphasizes the need for a quantum theory of gravity. As previously mentioned, modified gravity theories could provide valuable insights into the development of such a theory. This motivation is further strengthened by the realization that any attempt to unify particle physics with gravity inevitably requires some modification of Einstein's theory of gravity. Indeed, such modifications are almost dictated by the principles of quantum mechanics. If one starts with Einstein's gravity combined with particle fields at the tree level, quantum corrections will modify the gravitational interactions. These modifications result in interactions that are only finite if a cutoff is introduced, indicating that the theory, as it stands, is not renormalizable [70].

Therefore, when examining the early stages of the Universe, the notion of alternative descriptions of gravity beyond General Relativity can be justified by the aforementioned arguments. In fact, in this context, modified theories of gravity have provided valuable insights and made significant contributions to addressing the challenges associated with the primordial Universe. For instance, the initial singularity predicted by the Big Bang theory can be circumvented by proposing a cyclic cosmological model, where the Universe never contracts to a point of zero size—a theoretical outcome that some modified gravity theories support (that will be studied later on). Furthermore, one of the most notable achievements in this area, as previously mentioned, is the Starobinsky model of inflation [52]. This model, which is based on a Lagrangian of the form $\mathcal{L} = R + \frac{R^2}{M^2}$ (where M^2 is a constant with dimensions of mass), provides exceptionally accurate predictions for inflation [16]. A more detailed analysis of this model will be discussed in subsequent sections. Additionally, modified gravity has recently offered a promising solution to the lithium problem, demonstrating that this issue can be effectively addressed within the framework of $f(R)$ gravity theory [71].

Furthermore, the matter-antimatter asymmetry, arguably the most fundamental problem of the primordial Universe and the central focus of this thesis, can also be addressed through modifications to gravitational theory. Although this problem is typically explored through particle physics mechanisms and extensions of the Standard Model of particle physics, where gravity is considered only as a background framework, gravity itself could play a more central role and become a key component in these mechanisms. This idea is supported by the concept of gravitational baryogenesis [72], a mechanism that involves coupling the derivative of the Ricci scalar to the baryonic current, thereby providing a framework capable of generating the observed matter-antimatter asymmetry. While this mechanism has been successful within the context of GR, its limitations become apparent, prompting the exploration of this mechanism within the framework of modified theories of gravity. This approach has shown promising results and offers a potential path forward for addressing these shortcomings [73, 74, 75, 76, 77, 78, 79].

Moreover, since modifications to GR result in different expansion rates for the Universe that will have an impact on the interaction rates of particles, it becomes possible to consider combining mechanisms primarily developed within the framework of particle physics with these modified gravitational theories. This approach could potentially address existing problems and alleviate the constraints associated with these mechanisms.

With this being said, this thesis will explore ways to solve the asymmetry problem by exploring gravitational baryogenesis in the context of the modified theory of gravity $f(R,\mathcal{T}^2)$, with $\mathcal{T}^2$ being the contraction of the stress-energy tensor with itself, and with scalar-tensor theories, exploring how modifications to the expansion rate of the Universe can benefit two well-established baryogenesis mechanisms such as electroweak baryogenesis [80, 81, 82] and GUT baryogenesis [9, 83]. The links between modified gravity and inflation will also be exposed in a brief manner.

1.2 Differential geometry

As mentioned before, the mathematical framework behind General Relativity is manly built with differential geometry, a branch of mathematics dedicated to the study of the geometry of smooth shapes and smooth spaces, otherwise known as smooth manifolds. Additionally, many modified theories of gravity use also mathematical concepts of differential geometry. With such an important role, a good and cohesive introduction to this topic must be done. Therefore, in this section a brief exposition of differential geometry with only the basics and fundamentals will be done. Diverse books, lessons, and others materials exist when talking about differential geometry, but for this thesis, it was used the book [84] and the review paper [85] to construct this section. The subjects will be exposed in a physicist like manner aiming to expose the fundamentals with the necessary formalism.

1.2.1 The basics of topological spaces and manifolds

Differential geometry, more in specific for this study, Riemannian geometry is a complex subject that has tremendous tools for both mathematicians and physicists. It works profoundly with topology therefore demands a cohesive comprehension of topological notions, a complex subject. But as you usually do with difficult things, we will start with the fundamental and simplest part.

To begin with, a topological space is a mathematical framework that allows for the examination of properties of a space that remain unchanged under continuous transformations. Within this framework, two spaces are considered topologically equivalent if one can be transformed into the other through continuous deformation without tearing or joining. This concept holds significant importance in physics, as it can be applied to numerous physical systems capable of undergoing continuous changes without affecting their core properties, such as symmetries and internal relationships. This idea also underpins our understanding of spacetime. The four-dimensional reality we experience, termed "spacetime,"is described in classical physics as a ”four-dimensional continuum.” This implies that four coordinates are necessary to uniquely define events. In both pre-relativistic and special relativistic frameworks, it is assumed that there is a direct correspondence between events in spacetime and the topological space $\mathbb{R}^4$. From a practical viewpoint, the primary interest of physicists in studying topological spaces lies in the associated metric, which is used to measure distances between points. However, as expected, not all topological spaces have a metric associated. Additionally, considering that in physics most of the systems are dynamical and governed by a set of equations, if only any global properties of the system were assumed, such as its topology, this would limit the solutions to the equations that govern the system and would not allow to take into account a wealth of interesting physical phenomena. To obtain a complete description manifolds are introduced. In simple terms, manifolds, denoted by $\mathcal{M}$, are a subclass of topological spaces that are locally Euclidean[1]. This means that for each point $P \in \mathcal{M}$, there exists a neighborhood in which one can define a set of coordinates $\{x_\mu\}$ to specify points around it, much like in Euclidean space (for a better visualization imagine a sphere that when we zoom in a good amount we see a flat plane). Therefore, we can describe a manifold as a topological space that locally resembles Euclidean space $\mathbb{R}^n$. However, the global structure of a manifold can differ from $\mathbb{R}^n$, resulting in a space that exhibits more complex properties than those found in standard Euclidean space. Additionally, it is crucial to differentiate between the topological space $\mathbb{R}^n$ and the vector space $\mathbb{R}^n$. The topological space $\mathbb{R}^n$ allows for the discussion of points p and their local neighborhoods, focusing on spatial relationships and continuity. In contrast, the vector space $\mathbb{R}^n$ involves a set of points that adhere to specific algebraic rules, including operations such as vector addition and scalar multiplication. Essentially, while $\mathbb{R}^n$ as a topological space concerns itself with the structure of points and their proximities, introducing vector space axioms transforms these points into vectors $\vec{p}$, thereby endowing them with additional algebraic properties.

In sum, a manifold $\mathcal{M}$ can be understood as a space composed of points p. As a topological space, $\mathcal{M}$ has a well-defined concept of neighborhoods, enabling analysis of the local structure around a point p. Specifically, there exists a local homeomorphism, which is a mapping from $\mathcal{M}$ to $\mathbb{R}^n$ that preserves the topological structure locally. This mapping transforms the point p and its surrounding neighborhood into a point and its neighborhood in $\mathbb{R}^n$. Given the coordinate system in $\mathbb{R}^n$, where each point is uniquely

[1] To be slightly more precise, $\mathcal{M}$ is a **topological space** which is *locally homeomorphic* to the *topological* space $\mathbb{R}^n$ and more technically, a real n-dimensional manifold $\mathcal{M}$ is a real n-dimensional topological space which is Hausdorff, paracompact, and locally homeomorphic to n-dimensional Euclidean space $\mathbb{R}^n$.

identified by n coordinates, this process facilitates the assignment of coordinates to the points within $\mathcal{M}$. It is important to note that the assignment of coordinates is not unique. Although we typically label points in $\mathbb{R}^n$ using n numerical values, different individuals might choose distinct coordinate grids for this purpose. We represent a coordinate system by $\{x^\mu\}$ where x^μ is the μ-th coordinate. To connect one coordinate system to another, we utilize the concept of a coordinate transformation. This is actually a specific example of a broader concept known as a diffeomorphism ϕ, which is a smooth (infinitely differentiable) function $\phi : \mathcal{N} \to \mathcal{M}$ that maps one manifold $\mathcal{N}$ onto another manifold $\mathcal{M}$. In the case of a coordinate transformation, this diffeomorphism takes the form $\phi : \mathcal{M} \to \mathcal{M}$, meaning it maps the manifold $\mathcal{M}$ onto itself. Additionally, it must have a smooth inverse and relate the original coordinates $\{x^\mu\}$ to a new set of coordinates $\{x^\mu\} := \{\phi(x^\mu)\}$.

1.2.2 Vector Fields and Tensor Fields

The idea of dimensions is embedded in us and in our description of our Universe. With this notation, comes the idea of scalars, vectors and even tensors but how are these objects, or more in specific and fundamentally vector/tensor fields, related with topology? Starting with vectors (that usually are also called contravariant vectors), the fundamental idea is to realize that a vector allows us to define the directional derivative of scalar fields. This corresponds to the intuitive notion that a vector has a direction with an object which is intrinsically defined on the manifold, that in this case is a scalar $f : \mathcal{M} \to \mathbb{R}$. Formally, in a given coordinate system, $\{x^\mu\}$, one can write the directional derivative of f (in this coordinate system) as

$$v := v^\mu \partial_\mu \tag{1.1}$$

with $\partial_\mu \equiv \frac{\partial}{\partial x^\mu}$ being the basis vectors $\{e_\mu\}$ and where $v^\mu \in C^\infty(\mathcal{M})$ are n smooth functions of the coordinates. Additionally, we define the components of the vector field v with respect to a coordinate system $\{x^\mu\}$ as

$$v^\mu := v(x^\mu)\,, \tag{1.2}$$

that usually in physics we call the vector field (or contravariant vector sometimes - index raised). Before we move forward, it is helpful to introduce some key terminology and provide a slightly more abstract definition of tangent vectors. Recall that a vector field v is a function that maps smooth functions on the manifold, denoted as $C^\infty(\mathcal{M})$, to other smooth functions on the manifold, $C^\infty(\mathcal{M})$. A tangent vector at a point p is defined as a map v_p that takes smooth functions on the manifold, $C^\infty(\mathcal{M})$, to real numbers $\mathbb{R}$. This is done by evaluating the vector field v at the specific point $p \in \mathcal{M}$,

$$\begin{aligned} &v_p : C^\infty(\mathcal{M}) \to \mathbb{R} \\ &v_p(f) := v(f)|_p\,. \end{aligned} \tag{1.3}$$

Essentially, a tangent vector v_p at a point p is defined by applying the vector field v to a smooth function f and then evaluating the result at p, resulting in a real number. The set of all tangent vectors at the point p is referred to as the tangent space at p and is denoted by $T_p\mathcal{M}$. In addition to this, there is the concept of the tangent bundle, which can be informally understood as the collection of all tangent spaces across every point on the manifold $\mathcal{M}$. It is important to note that the tangent space at any point p, denoted $T_p\mathcal{M}$, is a real, n-dimensional vector space. This implies that for any two elements, such as

v_p and u_p in $T_p\mathcal{M}$, all operations that are valid for vectors in $\mathbb{R}^n$ can also be performed. Specifically, all elements in $T_p\mathcal{M}$ adhere to the rules of vector addition, scalar multiplication, and other vector space operations.

With this defined, the next fundamental concept is the concept of a covector (or 1-form in a more formal way or covariant vector sometimes - index lowered). Since $T_p\mathcal{M}$ is a real, n-dimensional vector space, it naturally has a corresponding real, n-dimensional dual space, denoted by $T_p^*\mathcal{M}$. This dual space is also known as the cotangent space at p and consists of linear functionals. A linear functional α can be described as a function that takes a vector as input and outputs a real number. Formally, this can be defined as the linear map

$$\alpha : T_p\mathcal{M} \to \mathbb{R} \tag{1.4}$$

$$v \to \langle \alpha, v \rangle \in \mathbb{R}, \tag{1.5}$$

where α is identified as a covector, and $\langle \cdot, \cdot \rangle$ represents the inner product of a 1-form with a vector (an inherent property). In a given coordinate system $\{x^\mu\}$, the components of α can be defined as

$$\alpha_\mu := \langle \alpha, \partial_\mu \rangle \,, \tag{1.6}$$

which means that these components are derived by evaluating the linear functional on the basis vectors of $T_p\mathcal{M}$. By α being a linear map, the expression for the pairing of v with α in terms of coordinates can be computed as

$$\langle \alpha, v \rangle = \langle \alpha, v^\mu \partial_\mu \rangle = v^\mu \langle \alpha, \partial_\mu \rangle = v^\mu \alpha_\mu \,,$$

where in the last it is implicit the Einstein summation convention, i.e., a sum due to repeated indices. The vector v is first expanded in terms of its basis, followed by applying the linearity of $\langle \cdot, \cdot \rangle$, and finally using the defined components of the covector. It's important to note that both vector fields and covectors fields are defined as linear maps. Additionally, in any coordinate system $\{x^\mu\}$, the basis covectors for $T_p^*\mathcal{M}$ can be defined as $\mathrm{d}x^\mu$, allowing to express the components of the dual-vector α as

$$\alpha = \alpha_\mu \, \mathrm{d}x^\mu. \tag{1.7}$$

where the basis covectors are required to satisfy the condition

$$\langle \mathrm{d}x^\mu, \partial_\nu \rangle = \delta^\mu_\nu \,, \tag{1.8}$$

with δ^μ_ν being the Kronecker delta to ensure consistency with the earlier definition and reproduce the coordinate pairing. By both vector fields and covectors fields being linear maps, one can employ a definition of more complex objects, such as tensors, as multilinear maps. A tensor of type (p,q) is defined as a multilinear map

$$H : (T\mathcal{M})^{\otimes p} \otimes (T^*\mathcal{M})^{\otimes q} \to \mathbb{R} \,, \tag{1.9}$$

with $^{\otimes p}$ representing $(T\mathcal{M})$ p times (and the same for $^{\otimes q}$ and that accepts p vectors and q covectors as arguments and returns a real number. This can also be represented as

$$H(v_1, \ldots, v_p, \alpha_1, \ldots, \alpha_q). \tag{1.10}$$

Due to the multilinearity property of H, in a coordinate system $\{x^\mu\}$, we can express it as

$$H(v_1, \ldots, v_p, \alpha_1, \ldots, \alpha_q) = v_1^{\mu_1} \cdots v_p^{\mu_p} (\alpha_1)_{\nu_1} \cdots (\alpha_q)_{\nu_q} H^{\mu_1 \cdots \mu_p}_{\nu_1 \cdots \nu_q} \,, \tag{1.11}$$

where the components of H are defined as

$$H^{\mu_1\cdots\mu_p}_{\nu_1\cdots\nu_q} = H(\partial_{\mu_1},\ldots,\partial_{\mu_p},\mathrm{d}x^{\nu_1},\ldots,\mathrm{d}x^{\nu_q}). \tag{1.12}$$

1.2.3 Transformations and Densities

The behaviour of vectors and covectors under coordinate changes is simple. A change of coordinates can be defined as a diffeomorphism that maps the original coordinates $\{x^\mu\}$ to new coordinates $\{\tilde{x}^\mu\}$. Given these two coordinate system, $\{\tilde{x}^\mu\}$ and $\{x^\mu\}$, a vector (and equally a covector) in the first coordinate system are related with the second coordinate system in the following way

$$v = v^\mu \partial_\mu = \tilde{v}^\nu \tilde{\partial}_\nu, , \tag{1.13}$$

where $\widetilde{v}^\mu$ are the components of v with respect to the vector basis $\partial/\partial\widetilde{x}^\mu$, in a new coordinate system $\widetilde{x}^\mu$ and $v^\mu \neq \tilde{v}^\nu$. Moreover, the inner product of a vector and a dual vector, given that 1-forms map vectors to real numbers in a coordinate-independent manner, is given by

$$\langle\alpha, v\rangle = \alpha_\mu v^\mu = \tilde{\alpha}_\nu \tilde{v}^\nu. \tag{1.14}$$

Although for vectors these transformations are simple, tensors, due to their multilinear nature, exhibit specific transformation behaviors under coordinate changes. Employing a more formal description, the transformation of partial derivatives under such a coordinate change can be written as

$$\frac{\partial}{\partial x^\mu} = \frac{\partial \tilde{x}^\lambda}{\partial x^\mu}\frac{\partial}{\partial \tilde{x}^\lambda} = J^\lambda_\mu \frac{\partial}{\partial \tilde{x}^\lambda}, \tag{1.15}$$

where J^λ_μ denotes the Jacobian matrix defined as

$$J^\lambda_\mu = \frac{\partial \tilde{x}^\lambda}{\partial x^\mu}. \tag{1.16}$$

This definitatons allows directely to obtain the results present in Eq.(1.13). Additionaly, given that the transformation $\tilde{x}^\mu(x)$ is a diffeomorphism, the Jacobian is non-degenerate, which ensures the existence of an inverse

$$(J^{-1})^\mu_\nu = \frac{\partial x^\mu}{\partial \tilde{x}^\nu}. \tag{1.17}$$

Finally, with these notations, by utilizing the multilinear properties of tensors, we can derive the transformation behavior for these objects as

$$\tilde{H}^{\mu_1\ldots\mu_p}{}_{\nu_1\ldots\nu_q} = J^{\mu_1}_{\omega_1}\cdots J^{\mu_p}_{\omega_p}(J^{-1})^{\beta_1}_{\nu_1}\cdots(J^{-1})^{\beta_q}_{\nu_q} H^{\omega_1\cdots\omega_p}_{\beta_1\cdots\beta_q}. \tag{1.18}$$

At this stage, it is useful to introduce the concept of tensor densities. A tensor density is a type of tensor (including scalar fields, which are tensors of type $(0,0)$) that does not transform in the usual manner but instead acquires a factor involving the determinant of the Jacobian matrix. A tensor density $\mathcal{K}$ of weight w transforms according to

$$\mathcal{K}^{\alpha_1\cdots\omega_p}_{\beta_1\cdots\beta_q} = (\det(J))^w (J^{-1})^{\omega_1}_{\mu_1}\cdots(J^{-1})^{\omega_p}_{\mu_p} J^{\nu_1}_{\beta_1}\cdots J^{\nu_q}_{\beta_q}\tilde{\mathcal{K}}^{\mu_1\ldots\mu_p}_{\nu_1\ldots\nu_q}, \tag{1.19}$$

where w is the density weight. This transformation highlights that a tensor density of weight zero is simply an ordinary tensor. Tensor densities play a crucial role in integrating over manifolds. To ensure that integrals constructed from tensorial quantities are independent of the coordinate system, the integrand must transform as a scalar density with weight $w = +1$.

1.2.4 (Pseudo-)Riemannian metric, affine connection and covariant derivative

The framework defined until this point is almost complete (at least for our interest) but still lacks two crucial capabilities. The first capability is the scalar product. We have primarily worked with the manifold $\mathcal{M}$ that is adequate for discussing various mathematical and physical concepts such as events, curves (which are used to model observers and test particles), scalar fields, vector fields, general tensor fields of type (p,q), and tensor densities. The notion of scalar product allows to known lengths of curves and magnitudes of vectors. To obtain such feat can be obtained with the metric tensor g. The metric serves as a generalization of the notion of scalar product between vectors from Euclidean geometry to any kind of geometry. In a formal way, the metric is defined as

$$\begin{aligned} g : T\mathcal{M} \times T\mathcal{M} &\to \mathbb{R} \\ (u,v) &\mapsto g(u,v) \end{aligned} \tag{1.20}$$

which satisfies the following axioms

A1 Symmetry: $g(\beta,\alpha) = g(\alpha,\beta)$,

A2 Linearity in both slots: $g(f\beta_1 + \beta_2, \alpha) = f g(\beta_1,\alpha) + g(\beta_2,\alpha)$
$g(\beta, f\alpha_1 + \alpha_2) = f g(\beta,\alpha_1) + g(\beta,\alpha_2)$,

A3 Non-degeneracy: If $g(\beta,\alpha) = 0$ for all $\alpha = 0$, then $\beta = 0$.

The metric tensor is fundamentally a function that takes two vectors as inputs and returns a real number. When provided with a coordinate chart $\{x^\mu\}$ and a basis $\{e_\mu\}$ of the tangent space $T\mathcal{M}$, the components of the metric tensor g in that particular chart and basis can be defined as

$$g_{\mu\nu} \coloneqq g(e_\mu, e_\nu)\,. \tag{1.21}$$

According to axiom A1, we have $g_{\mu\nu} = g_{\nu\mu}$, indicating that the metric tensor is symmetric. Axiom A3 ensures the existence of an inverse metric, denoted by $g^{\mu\nu}$. The metric tensor and its inverse satisfy the important relation $g_{\mu\kappa}g^{\kappa\nu} = \delta^\mu_\nu$. An additional important point of metrics is the nomenclature used. Physicists, besides calling $g_{\mu\nu}$ as metric, often also refer to $\mathrm{d}s^2 = g_{\mu\nu}\,\mathrm{d}x^\mu \mathrm{d}x^\nu$ as a "metric". However, if we adhere more strictly to mathematical definitions, the metric is more accurately described as a tensor, denoted by $g = g_{\mu\nu}\,\mathrm{d}x^\mu \otimes \mathrm{d}x^\nu$. This tensor formalism captures the full, coordinate-independent nature of the metric. Nonetheless, in this thesis, we will also refer to $\mathrm{d}s^2$ as a metric. This expression, $\mathrm{d}s^2$, represents the line element or the squared infinitesimal distance between two points in the manifold and is a commonly used shorthand in physics to describe the geometry encoded by the metric tensor g. By allowing this notation, we maintain consistency with the terminology frequently used in physical literature, while still aligning with the more precise mathematical definitions when necessary.

By utilizing axiom A2, we can further express $g(v,w)$ as

$$g(v,w) = g(v^\mu e_\mu, w^\nu e_\nu) \overset{\text{A2}}{=} v^\mu g(e_\mu, w^\nu e_\nu) \overset{\text{A2}}{=} v^\mu w^\nu g(e_\mu, e_\nu) = g_{\mu\nu} v^\mu w^\nu\,. \tag{1.22}$$

Additionally, it is possible to establish an isomorphism between $T_p\mathcal{M}$ and $T_p^*\mathcal{M}$ through the metric

$$\alpha_\mu = g_{\mu\nu}\alpha^\nu \equiv \alpha_\mu \ , \quad v^\mu = g^{\mu\nu}v_\nu \equiv v^\mu \, , \tag{1.23}$$

so the metric can be understood as a way to lower and raise indices.

This framework extends the familiar concept of the scalar product between vectors from Euclidean geometry to more general geometric contexts as previously mentioned. Given a metric tensor g, we can define not only the norm of vectors but also the angles between them, as well as compute areas, volumes, and other geometric quantities. For instance, the norm of a vector v is defined as

$$\|v\|^2 := g(v,v) = g_{\mu\nu}v^\mu v^\nu = v_\nu v^\nu \, . \tag{1.24}$$

It's no surprise that the metric has an intrinsic relation with the manifold as a specific metric "defines"what type of manifold is at question. For example, if a differentiable manifold $\mathcal{M}$ admits a Riemannian metric, then $\mathcal{M}$ is called a Riemannian manifold. In a Riemannian metric, all eigenvalues are positive, reflecting its positive-definite nature. In contrast, a pseudo-Riemannian metric includes both positive and negative eigenvalues. The count of positive eigenvalues $i > 0$ and negative eigenvalues $j < 0$ defines the index of the pseudo-Riemannian metric, denoted as the pair (i, j). A pseudo-Riemannian metric with exactly one negative eigenvalue ($j = 1$) is referred to as a Lorentzian metric, characterized by the index $(i, 1)$. When a manifold $\mathcal{M}$ is equipped with a Lorentzian metric, it is termed a Lorentzian manifold. A quintessential example of a Lorentzian metric is the Minkowski metric, expressed as $(\eta_{\mu\nu}) = \mathrm{diag}(-1, 1, 1, 1)$, which represents the flat spacetime of special relativity. Correspondingly, a 4-dimensional Minkowski space(-time) serves as a standard example of a Lorentzian manifold. The use of Lorentzian manifolds to model spacetime is motivated by the observation that time and space are experienced differently; therefore, assigning different signs to the temporal and spatial components of the metric aligns with this distinction. For the remainder of this discussion, we shall focus on 4-dimensional Lorentzian manifolds. Hereafter, the metric tensor will be denoted by $g_{\mu\nu}$ to differentiate it from its determinant, which will be referred to as g.

Additionally, in contexts where Lorentzian metrics are used, such as in relativity, vectors can be classified based on their norms as **spacelike**, **timelike**, or **null**. Specifically, a vector v is considered

$$v \text{ is called } \begin{cases} \textbf{spacelike} & \text{if } g(v,v) > 0\,, \\ \textbf{null} & \text{if } g(v,v) = 0\,, \\ \textbf{timelike} & \text{if } g(v,v) < 0\,. \end{cases} \tag{1.25}$$

This classification relies on the assumption that the signature of g is mostly positive. If we were to define the signature of a Lorentzian metric as $(1, n-1)$, the conditions involving $>$ and $<$ would be reversed for even n. However, these definitions are consistent across both conventions when the number of dimensions n is odd.

This classification of vectors can be extended to curves and hypersurfaces as well. A curve γ is classified as

$$\gamma \text{ is } \begin{cases} \text{spacelike} & \text{if its } \textbf{tangent} \text{ vector is everywhere spacelike,} \\ \text{null} & \text{if its } \textbf{tangent} \text{ vector is everywhere null,} \\ \text{timelike} & \text{if its } \textbf{tangent} \text{ vector is everywhere timelike.} \end{cases} \tag{1.26}$$

With the metric defined, the second notion that we need is an object that can determine the change of a vector along a curve on $\mathcal{M}$. This object is referred to as an affine connection, and it serves to link nearby tangent spaces $T_p\mathcal{M}$. The affine connection enables the differentiation of vector fields on a manifold $\mathcal{M}$ in a manner analogous to the differentiation of scalar functions.

To define it, lets start by considering a Lorentzian manifold $\mathcal{M}$. In this curved spacetime, even the basis vectors change as one moves along a curve on $\mathcal{M}$. This variation is captured by the connection coefficients, denoted as $\Gamma^{\alpha}_{\mu\nu}$, which are defined by

$$\partial_\mu e_\nu = \Gamma^{\alpha}_{\mu\nu} e_\alpha \,. \tag{1.27}$$

In general, the connection coefficients of a Lorentzian manifold can be written as

$$\Gamma^{\alpha}_{\mu\nu} = \left\{ {}^{\alpha}_{\mu\nu} \right\} + K^{\alpha}{}_{\mu\nu}. \tag{1.28}$$

where $\left\{ {}^{\alpha}_{\mu\nu} \right\}$ are the Christoffel symbols, which are defined as

$$\left\{ {}^{\alpha}_{\mu\nu} \right\} \equiv \frac{1}{2} g^{\alpha\lambda} \left(\partial_\mu g_{\nu\lambda} + \partial_\nu g_{\mu\lambda} - \partial_\lambda g_{\mu\nu} \right), \tag{1.29}$$

and $K^{\alpha}{}_{\mu\nu}$ is the contorsion tensor, which is defined as

$$K^{\alpha}{}_{\mu\nu} \equiv \frac{1}{2} \left(T^{\alpha}{}_{\mu\nu} + T_{\mu}{}^{\alpha}{}_{\nu} + T_{\nu}{}^{\alpha}{}_{\mu} \right) \,. \tag{1.30}$$

The contorsion tensor is defined in terms of the torsion tensor, whose definition is

$$T^{\alpha}_{\mu\nu} \equiv \Gamma^{\alpha}_{\mu\nu} - \Gamma^{\alpha}_{\nu\mu}. \tag{1.31}$$

Utilizing now definition (1.27), one can show that the differentiation of a vector field $v = v^\nu e_\nu$ proceeds as follows

$$\partial_\mu \left(v^\nu e_\nu \right) = \left(\partial_\mu v^\nu \right) e_\nu + v^\nu \partial_\mu e_\nu = \left(\partial_\mu v^\nu + \Gamma^{\nu}_{\mu\alpha} v^\alpha \right) e_\nu. \tag{1.32}$$

This formulation highlights how the connection coefficients $\Gamma^{\nu}_{\mu\alpha}$ account for the changes in both the components v^ν of the vector field and the basis vectors e_ν themselves, providing a way to perform differentiation in a curved space, beyond the straightforward differentiation of functions in flat space. Therefore, without much formalism, we can define the covariant derivative of contravariant vector V^ν as

$$\nabla_\mu v^\nu \equiv \partial_\mu v^\nu + \Gamma^{\nu}_{\mu\alpha} v^\alpha, \tag{1.33}$$

The covariant derivative serves to extend the concept of the partial derivative from flat spaces, where the basis vectors are uniform and do not vary from one point to another, to curved manifolds, where this is no longer the case. In flat spaces, differentiation is straightforward because the coordinate system remains unchanged. However, on a curved manifold, the coordinate basis vectors change from point to point, and thus, a more refined notion of differentiation is needed. The covariant derivative compensates for the variability of the basis vectors, allowing for the consistent differentiation of tensor fields across the manifold.

When defining the covariant derivative of a covector (or dual-vector or 1-form), a similar construction is used, but with a crucial difference: the connection term appears with a negative sign (for a full deduction see [84, 85]). This difference ensures that the derivative of the covector properly reflects the geometry of the space, maintaining consistency with the fundamental properties of tensor fields and their transformations under coordinate changes. Thus, for a covector the covariant derivative is given by

$$\nabla_\mu \alpha_\nu \equiv \partial_\mu \alpha_\nu - \Gamma^\kappa_{\mu\nu}\alpha_\kappa. \tag{1.34}$$

Generalizing for tensors with arbitrary covariant and contravariant indices, one has

$$\nabla_\alpha T^{\mu_1\dots\mu_p}_{\nu_1\dots\nu_q} = \partial_\alpha T^{\mu_1\dots\mu_p}_{\nu_1\dots\nu_q} + \Gamma^{\mu_1}_{\alpha\lambda} T^{\lambda\dots\mu_p}_{\nu_1\dots\mu_q} + \cdots + \Gamma^{\mu_p}_{\alpha\lambda} T^{\mu_1\dots\lambda}_{\nu_1\dots\nu_q} - \Gamma^{\lambda}_{\alpha\nu_1} T^{\mu_1\dots\mu_p}_{\lambda\dots\nu_q} - \cdots - \Gamma^{\lambda}_{\alpha\nu_q} T^{\mu_1\dots\mu_p}_{\nu_1\dots\lambda}. \tag{1.35}$$

Given that we are considering a Lorentzian manifold, which is a differentiable manifold equipped with a metric, certain conditions can be imposed on the connections we work with. A natural constraint is to require the metric tensor $g_{\mu\nu}$ to be covariantly constant. This condition implies that the norm of a vector or, equivalently, the inner product between two vectors, remains unchanged under parallel transport. Mathematically, this requirement is expressed as

$$\nabla_\alpha g_{\mu\nu} = 0\,, \tag{1.36}$$

which is known as the metricity condition. When a connection satisfies this condition, it is referred to as a metric connection.

Additionally, if we impose that the connection coefficients are symmetric in their lower indices,

$$\Gamma^\alpha_{\mu\nu} = \Gamma^\alpha_{\nu\mu}\,, \tag{1.37}$$

we ensure, according to Eq. (1.31), that the torsion tensor vanishes. Consequently, this also implies that the contorsion tensor is zero. Under these conditions, the connection coefficients, or Christoffel symbols, take the following form

$$\Gamma^\alpha_{\mu\nu} = \frac{1}{2} g^{\alpha\lambda}\left(\partial_\mu g_{\nu\lambda} + \partial_\nu g_{\mu\lambda} - \partial_\lambda g_{\mu\nu}\right). \tag{1.38}$$

The resulting affine connection is known as the Levi-Civita connection. This result aligns with the fundamental theorem of Riemannian geometry, which asserts that on any (pseudo-)Riemannian manifold, there exists a unique affine connection that is both torsion-free and compatible with the metric. This unique connection is precisely the Levi-Civita connection, characterized by the Christoffel symbols.

1.2.5 Integrating over manifolds

The last important tool to define and explore is integration over manifolds. Considering an m-dimensional Lorentzian manifold $\mathcal{M}$, there exists a volume element that remains unchanged under coordinate transformations. Mathematically this can be overseen but in physics, this property is particularly significant when developing physical theories, as it ensures that the laws of physics are expressed in a form that is consistent and independent of the chosen coordinate system. The invariance of the volume element under such transformations is essential because it allows for a formulation of physical laws that are universally applicable throughout the manifold. Thus, the volume element plays a vital role in maintaining the general covariance of physical theories, reinforcing the principle that the laws of nature should hold true universally, regardless of location or coordinate choice.

Tensor densities are crucial for performing integration on manifolds in a way that respects coordinate independence. To ensure that an integral remains consistent regardless of the coordinate system used for representing and performing the integration, the integrand must transform as a scalar density with a weight of $w = +1$. For instance, the square root of the determinant of the metric tensor, $\sqrt{-g}$, is a tensor density with weight $w = +1$. Therefore, we can now define the invariant volume element as

$$\Omega_{\mathcal{M}} \equiv \sqrt{-g}\mathrm{d}x^1\mathrm{d}x^2\ldots\mathrm{d}x^m\,, \tag{1.39}$$

By working in a four-dimensional space-time one can use Eq.(1.39) to define an integration of an arbitrary function f over all space-time leading to

$$\int_{\mathcal{M}} f\Omega_{\mathcal{M}} \equiv \int_{\mathcal{M}} \sqrt{-g} f \mathrm{d}^4x. \tag{1.40}$$

The physical meaning of this integration comes from f. One can substitute the f function by the Lagrangian of a gravitational theory, $\mathcal{L}$, and define its correspondent action by

$$S \equiv \int_{\mathcal{M}} \mathcal{L}\Omega_{\mathcal{M}} = \int_{\mathcal{M}} \sqrt{-g}\mathcal{L}\mathrm{d}^4x\,, \tag{1.41}$$

defining therefore a fundamental framework. In physics, actions are fundamental as they provide the basis for deriving the field equations that govern the dynamics of a theory. A critical tool for integration on manifolds, especially Lorentzian manifolds, is the generalized Stokes' Theorem. This theorem is expressed as

$$\int_{\mathcal{M}} \mathrm{d}\omega = \int_{\partial\mathcal{M}} \omega, \tag{1.42}$$

where ω represents a differential form, $\mathrm{d}\omega$ denotes its exterior derivative, and $\partial\mathcal{M}$ signifies the boundary of the manifold $\mathcal{M}$. This theorem generalizes familiar vector calculus theorems and plays a crucial role in deriving field equations.

1.2.6 Curvature

Working with spaces that usually are curved, it is important to consider how the direction of a vector changes under parallel transport, a way of transporting geometrical quantities along smooth curves in a manifold. Indeed such consideration leads to one of the most important concepts in differential geometry, curvature. To describe and quantify curvature in curves and surfaces, one has to introduce the Riemann curvature tensor that can be expressed in terms of the Christoffel symbols as

$$R^{\alpha}_{\beta\mu\nu} = \partial_\mu\Gamma^{\alpha}_{\beta\nu} - \partial_\nu\Gamma^{\alpha}_{\beta\mu} + \Gamma^{\alpha}_{\mu\lambda}\Gamma^{\lambda}_{\beta\nu} - \Gamma^{\alpha}_{\nu\lambda}\Gamma^{\lambda}_{\beta\mu}\,. \tag{1.43}$$

This tensor has important properties, called the Bianchi identities. These identities are relations between the covariant derivatives of the components of the Riemann tensor, and are expressed as

$$\nabla_\lambda R^{\alpha}_{\beta\mu\nu} + \nabla_\nu R^{\alpha}_{\beta\lambda\mu} + \nabla_\mu R^{\alpha}_{\beta\nu\lambda} = 0. \tag{1.44}$$

Additionally, one of the traces of the Riemann tensor is the Ricci tensor given by

$$R_{\mu\nu} \equiv R^{\alpha}_{\mu\alpha\nu}. \tag{1.45}$$

that gives a more compact and simple representation of the curvature of a Riemannian manifold. In physics, it describes how does the space-time volume of an object varies due to gravitational tides. At last the trace of Ricci tensor gives the Ricci scalar

$$R = g^{\mu\nu} R_{\mu\nu}\,, \tag{1.46}$$

a quantity particularly significant in curvature-based theories of gravity as it offers a way to quantify the average curvature of spacetime without the computational complexity associated with a rank-4 tensor and, being a scalar, it remains invariant under Lorentz transformations, making it an ideal candidate for inclusion in the gravitational action.

With these three quantities defined, one can obtain the contract Bianchi identities by using Eq (1.44) and Eq. (1.36), giving

$$\nabla^{\mu} R_{\mu\nu} = \frac{1}{2}\nabla_{\nu} R\,, \tag{1.47}$$

which can be equivalently expressed as

$$\nabla^{\mu}\left(R_{\mu\nu} - \frac{1}{2} g_{\mu\nu} R\right) = 0\,, \tag{1.48}$$

where it is defined

$$G_{\mu\nu} \equiv R_{\mu\nu} - \frac{1}{2} g_{\mu\nu} R\,, \tag{1.49}$$

as the Einstein tensor.

1.3 General Relativity from the variational principle

There are numerous methods to derive GR field equations, but one particularly prominent approach is through the action principle, specifically the variational principle. This method was introduced in the context of GR by David Hilbert [86] (the man who almost beat Einstein in the race to deduce GR field equations), who sought to formulate the theory's Lagrangian framework. Today, deriving the Einstein field equations through the action principle is the preferred method, as it requires only the theory's Lagrangian. This approach proves particularly useful when exploring modified theories of gravity, as one starts with an assumed Lagrangian or action, and the variational principle directly yields the modified field equations. We will derive the Einstein field equations using this variational approach as the main ideas and results from this derivation will be of use in the following sections.

There are two foundational principles, fundamental two GR, that also motivated this method: the principle of general covariance and the equivalence principle. The first asserts that the laws of physics must maintain the same form in all coordinate systems. In contrast, the equivalence principle posits that in a specific coordinate system, the effects of gravity can be locally negated. In addition to these principles, GR must also satisfy the requirement that, in the weak-field limit, it approximates Newton's theory of gravitation. For a gravitational scalar potential Φ that corresponds to a matter density ρ, this potential satisfies the Poisson equation

$$\Delta\Phi = 4\pi G\rho, \tag{1.50}$$

where Δ denotes the Laplacian operator, and G is the gravitational constant. In GR, the gravitational potential Φ is substituted by the metric tensor components $g_{\mu\nu}$, which serve as the primary field of the theory. Instead of a mass density ρ, the theory uses the energy-momentum tensor $T_{\mu\nu}$ to describe matter's dynamics in spacetime. The corresponding field equations in GR, known as Einstein's field equations, are given by

$$R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R = \frac{8\pi G}{c^4}T_{\mu\nu}, \tag{1.51}$$

where c is the speed of light in a vacuum. The gravitational coupling constant $8\pi G/c^4$ ensures that in the limit of weak gravitational fields, Equation (1.51) simplifies to the Poisson equation (1.50).

With this in mind, lets start with the variational principle derivation. Lets begging by the simple, the vacuum. Considering this, the GR Lagrangian responsible for obtaining the field equations will only have a component responsible for the geometric part. By the metric tensor being considered as the field that mediates the gravitational interaction, the geometric Lagrangian has to contain a dependence on derivatives of the metric, in order to describe its dynamics. The simplest scalar that satisfies this condition is the Ricci scalar. Therefore, the geometric Lagrangian should be proportional to it so the vacuum field equations can with

$$\mathcal{L}_{\rm g} = \frac{c^4}{16\pi G}R, \tag{1.52}$$

where the constant factor appears to reproduce the Newtonian limit in the presence of matter, giving the action

$$S_{\rm EH} \equiv \frac{c^4}{16\pi G}\int_{\mathcal{M}} \sqrt{-g}\, R\, {\rm d}^4x, \tag{1.53}$$

where $\mathcal{M}$ is a 4-dimensional Lorentzian manifold with a Lorentzian metric $g_{\mu\nu}$ that has a determinant g and on which one defines a set of coordinates $\{x^\mu\}$ as usual.

Employing now the concept of action principle, to derive the motion equations of a given theory, by means of the variational principle, one have to perform independent variations with respect to the fields that enter the action. Therefore, we must vary it respect to the inverse metric applying $\delta S_{\rm EH} = 0$, in other words, by requiring vanishing of the variation. Doing such, Eq.(1.53) becomes

$$\delta S_{\rm EH} \equiv \frac{c^4}{16\pi G}\int_{\mathcal{M}} \delta\left(\sqrt{-g}g^{\mu\nu}R_{\mu\nu}\right)\, {\rm d}^4x\,. \tag{1.54}$$

To give a more comprehensive demonstration, lets explore how the each quantity is affected by the variation. Applying the product rule one has

$$\delta(\sqrt{-g}g^{\mu\nu}R_{\mu\nu}) = \delta(\sqrt{-g}g^{\mu\nu})R_{\mu\nu} + \sqrt{-g}g^{\mu\nu}\delta R_{\mu\nu}\,. \tag{1.55}$$

Starting by the last term of the previous equation. The variation of the Ricci scalar is given by

$$\delta R_{\mu\nu} = \nabla_\alpha \delta\Gamma^\alpha_{\mu\nu} - \nabla_\nu \delta\Gamma^\alpha_{\mu\alpha}, \tag{1.56}$$

that corresponds to the well known Palatini identity resulting in

$$\sqrt{-g}g^{\alpha\beta}\delta R_{\alpha\beta} = \nabla_\kappa[\sqrt{-g}(g^{\alpha\beta}\delta\Gamma^\kappa_{\alpha\beta} - \delta^\kappa_\beta g^{\alpha\beta}\delta\Gamma^\kappa_{\alpha\kappa})] = \partial_\kappa[\sqrt{-g}(g^{\alpha\beta}\delta\Gamma^\kappa_{\alpha\beta} - \delta^\kappa_\beta g^{\alpha\beta}\delta\Gamma^\kappa_{\alpha\kappa})]\,, \tag{1.57}$$

where it was used the metricity condition (1.36). This quantity is a covariant divergence of a vector so by the Stokes's theorem (1.42) this vanishes when integrated over the invariant volume element and hence it does not contribute to the field equations, thus we do not need to incorporate it in the final result of the variation.

The second term gives

$$\delta(\sqrt{-g}g^{\mu\nu})R_{\mu\nu} = \sqrt{-g}\delta g^{\alpha\beta}R_{\alpha\beta} - \frac{1}{2}\sqrt{-g}g_{\alpha\beta}R\delta g^{\alpha\beta} = \sqrt{-g}\delta g^{\alpha\beta}(R_{\alpha\beta} - \frac{1}{2}g_{\alpha\beta}R)\,, \tag{1.58}$$

where it was used

$$\delta\sqrt{-g} = -\frac{1}{2}\sqrt{-g}g_{\mu\nu}\delta g^{\mu\nu}\,. \tag{1.59}$$

With this simplifications done we can look again to the Eq.(1.54) we can now write

$$\delta S_{\mathrm{EH}} = \frac{c^4}{16\pi G}\int_{\mathcal{M}}\sqrt{-g}\delta g^{\mu\nu}\left[R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R\right]\,\mathrm{d}^4x = 0\,, \tag{1.60}$$

that, by using the action principle that states that for an arbitrary variation of the metric tensor, $\delta g^{\mu\nu}$, the quantity inside the brackets of Eq.(1.60) must be zero, allows to obtain the following field equations

$$R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R = 0\,, \tag{1.61}$$

where usually it is defined the Einstein tensor as

$$G_{\mu\nu} \equiv R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R\,. \tag{1.62}$$

Incorporating matter, corresponds to consider a Lagrangian responsible for the matter sector

$$\mathcal{L}_{\mathrm{m}} = \mathcal{L}_{\mathrm{m}}\left(g_{\mu\nu},\Psi\right)\,, \tag{1.63}$$

that is considered to be a function of the metric tensor and of a collection of possible non-gravitational matter fields, Ψ.

The density Lagrangian of matter, when varied gives

$$\delta\left(\sqrt{-g}\mathcal{L}_{\mathrm{m}}\right) = \frac{1}{\sqrt{-g}}\frac{\delta\left(\sqrt{-g}\mathcal{L}_{\mathrm{m}}\right)}{\delta g^{\mu\nu}}\sqrt{-g}\delta g^{\mu\nu}\,, \tag{1.64}$$

that allows to defined the energy-momentum tensor as

$$T_{\mu\nu} \equiv -\frac{2}{\sqrt{-g}}\frac{\delta\left(\sqrt{-g}\mathcal{L}_{\mathrm{m}}\right)}{\delta g^{\mu\nu}}\,, \tag{1.65}$$

where we enforce the condition that L_m depends only on the metric components, and not on their derivatives.

Combining then the geometric part and the matter sector Lagrangians and famous Gibbons-Hawking-York (GHY) boundary term [87, 88], a term that is necessary whenever the manifold $\mathcal{M}$ has a boundary $\partial\mathcal{M}$, otherwise the variational principle is ill-defined and would not give any field equations (for further details see [89, 90, 91]), the GR action is given by

$$S_{GR}[g,\Psi] = S_{EH}[g] + S_{GHY}[h] + S_{matter}[g,\Psi] \tag{1.66}$$

$$= \frac{c^4}{16\pi G}\int_{\mathcal{M}}\mathrm{d}^4x\sqrt{-g}\,(R-2\Lambda) + S_{matter}[g,\Psi] + \frac{c^4}{16\pi G}\oint_{\partial\mathcal{M}}\mathrm{d}^3y\sqrt{|h|}\,\varepsilon\,\mathcal{K}\,. \tag{1.67}$$

In this context, the cosmological constant, Λ, was introduced due to its importance. The parameter ε is defined as $\varepsilon = n_\mu n^\mu = \pm 1$, where n^μ represents the unit normal vector to the boundary $\partial\mathcal{M}$. This normal vector is normalized such that $\varepsilon = +1$ when $\partial\mathcal{M}$ is a timelike hypersurface, and $\varepsilon = -1$ when $\partial\mathcal{M}$ is a spacelike hypersurface. Here, h denotes the determinant of the metric induced on the boundary $\partial\mathcal{M}$, while $\mathcal{K}$ signifies the trace of the extrinsic curvature of $\partial\mathcal{M}$, considered as a hypersurface embedded within the manifold $\mathcal{M}$. The GHY term is necessary whenever the manifold M has a boundary $\partial\mathcal{M}$. In this thesis we will not attend to or be bothered by boundary terms as it is beyond the scope of this work. Thus, to obtain the field equations with matter we do the previous procedure using the derived results giving the varied action

$$\delta S_{\mathrm{GR}} = \frac{1}{2\kappa}\int_{\mathcal{M}}\sqrt{-g}\left[R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R + \kappa^2\frac{2}{\sqrt{-g}}\frac{\delta\left(\sqrt{-g}\mathcal{L}_{\mathrm{m}}\right)}{\delta g^{\mu\nu}}\right]\delta g^{\mu\nu}\mathrm{d}^4x\,, \tag{1.68}$$

resulting in

$$R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R = \kappa T_{\mu\nu}\,, \tag{1.69}$$

with $\kappa \equiv 8\pi G = M_{Pl}^{-2}$ with M_{Pl} being the Planck mass. An important result can be obtained by taking the divergence of Eq. (1.69) and using the Bianchi identities (1.48), one obtains the conservation equation of GR

$$\nabla^{\mu}T_{\mu\nu} = 0\,. \tag{1.70}$$

This conservation corresponds to the vanishing of the covariant divergence of the energy-momentum tensor of matter, implying that the energy-momentum tensor is conserved. A direct implication this result is the diffeomorphism invariance of General Relativity [92]. Alternatively, the vanishing of the covariant divergence of the energy-momentum tensor of matter can be interpreted as indicating that there is no transfer of energy and momentum between geometry and matter. Consequently, GR does not provide a suitable framework for studying irreversible matter creation from gravitational fields. These results and ideas will be fundamental when talking about modified theories of gravity.

The last point important to address in the section is the consideration of which fundamental field(s) is/are to be considered in the theory and consequently when using the variational principle. In the deduction where made it was assumed that the metric was the fundamental field of GR, which means that this field is responsible for mediating the gravitational interaction, being called the metric formalism. However, this isn't necessarily the only possible "true"consideration. For example, why couldn't we also assumed that the affine-connection was a fundamental field? This corresponds to the Palatini formalism [93] that treats the metric and the affine connections independently. Although for GR both formalism give the same results, when considering alternative descriptions and modifications to GR this fact does not hold. There are three different formalisms [85, 64], the two previously mentioned and the metric-affine. This formalism assumes also that the metric and the affine connections are independent of each other like the Palatini formalism, but considers that the matter Lagrangian depends also on the connections. In this work it will only be considered the metric formalism.

Chapter 2

Standard Cosmology in the Primordial Universe

Starting this thesis by introducing the current framework for cosmology with an emphasis on the primordial description seems counter-intuitive as the objective of this thesis is to explore changes to such cosmological description. Although given that the objective of this thesis is to explore modifications to the standard cosmological model, it is important an introduction to the current state of the art. This introduction not only encapsulates how modifications to gravity can alter standard cosmology but also provides a foundation that will be valuable throughout the thesis.

2.1 Fundamentals

In a brief manner, the Standard Cosmology Model (SCM) is characterized by General Relativity and the Cosmological Principle where GR serves to dictate the field equations to be used connecting the geometric description of space-time with the non-gravitational fields, and the Cosmological Principle declares which metric (the quantity responsible for characterizing the gravitational field) is adequate to describe our Universe at larges scales. As previously seen, the Einstein field equations can be derived from the action

$$S = \int d^4x\sqrt{-g}\left[\frac{1}{2\kappa}(R-2\Lambda)+\mathcal{L}_m\right] , \tag{2.1}$$

where $\sqrt{-g}\,\mathcal{L}_m$ is the Lagrangian density for the matter fields. As seen in the last section, by varying this action with respect to the inverse metric, $g^{\mu\nu}$, one obtains the following field equations

$$R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} + \Lambda g_{\mu\nu} = \kappa T_{\mu\nu} , \tag{2.2}$$

where $T_{\mu\nu}$ is the energy momentum-tensor of the matter fields defined as in (1.65).

With regard to the cosmological principle, it states that our Universe at sufficient large scales is homogeneous and isotropic (a logical assumption given the realization of inflation) leading to the use of the Friedmann-Lemaître-Robertson-Walker (FLRW) metric to describe our Universe. This metric is expressed as follows [94, 95]

$$\mathrm{d}s^2 = -\mathrm{d}t^2 + a^2(t)\left[\frac{\mathrm{d}r^2}{1-kr^2} + r^2(\mathrm{d}\theta^2 + \sin^2\theta\,\mathrm{d}^2\phi)\right] , \tag{2.3}$$

where $a(t)$ is the scale factor of the Universe, and r, θ, and ϕ represent spatial comoving coordinates, with r as the radial coordinate and θ and ϕ as spherical angular coordinates. The curvature parameter k can take values of -1, 0, or $+1$, corresponding to a Universe with negative, zero (flat), or positive curvature, respectively. Throughout this work, the metric signature convention used is $(-,+,+,+)$.

Additionally, for the matter sector, we assume an energy-momentum tensor that is consistent with the symmetries of the FLRW metric, given by [94]

$$T_{\mu\nu} = (\rho + p)u_\mu u_\nu + p g_{\mu\nu} \ , \tag{2.4}$$

where ρ represents the energy density of the Universe's matter content, and p is the isotropic pressure. This form of the energy-momentum tensor corresponds to that of a perfect fluid. Substituting this tensor into the Einstein field equations (2.2), and considering the FLRW metric (2.3), yields the following dynamical equations

$$H^2(t) + \frac{k}{a^2(t)} = \frac{\kappa}{3}\rho + \frac{\Lambda}{3} \, , \tag{2.5}$$

$$\dot{H}(t) + H^2(t) = -\frac{\kappa}{6}(\rho + 3p) + \frac{\Lambda}{3} \, , \tag{2.6}$$

where $H \equiv \dot{a}(t)/a(t)$ is the expansion rate of the Universe, with the overdot indicating a derivative with respect to cosmic time t. Equation (2.5) is known as the Friedmann equation and is derived from the 00 component of Einstein's field equations. On the other hand, Eq. (2.6) is the Raychaudhuri equation, which describes the acceleration of the Universe and is obtained by subtracting the Friedmann equation from the $i-i$ components of the Einstein field equations. Furthermore, these equations can be used alongside the conservation equation, which results from the fact that the Einstein tensor, $G_{\mu\nu}$, satisfies the contracted Bianchi identities, leading to the conservation of the energy-momentum tensor, i.e., $\nabla_\mu T^{\mu\nu} = 0$. The conservation equation is given by

$$\dot{\rho} = -3H(t)(\rho + p) \ , \tag{2.7}$$

which stems from the conservation of energy and is inherent in the structure of the gravitational field equations. To complete the system of equations governing the evolution of the scale factor, an appropriate barotropic equation of state is introduced, i.e., $p = w\rho = (\gamma - 1)\rho$. For all components, the simplest equation of state is provided by

$$\sum_i p_i = \sum_i (\gamma_i - 1)\rho_i \ , \tag{2.8}$$

where γ_i is a constant parameter, and $\gamma_i - 1$ represents the speed of sound, v_s^2, in the fluid i characterizing the i-th component of the Universe's matter content. This equation of state allows the integration of the energy conservation equation (2.7), leading to

$$\rho(t) = \sum_i \rho_{i,0} \left(\frac{a(t)}{a_0}\right)^{-3\gamma_i} = \sum_i \rho_{i,0}(1+z)^{-3\gamma_i} \ , \tag{2.9}$$

where $\rho(t) \equiv \sum_i \rho_i(t)$ represents the total energy density of the Universe at a given time t, and $\rho_{i,0} \equiv \rho_i(t_0)$ and $a_0 \equiv a(t_0)$ are integration constants, which, without loss of generality, can be set to the values of each component i of the Universe's matter content and the scale factor's present-day value, $t = t_0$. The set of equations (2.5), (2.6) and (2.7) make the fundamental framework of cosmology as they dictate the overall evolution of the Universe.

2.1.1 Evolution of the Universe from the Friedmann equations

To study the time evolution of the Universe, or the dynamic behavior of the scale factor, the history of the Universe is often divided into several cosmological epochs, each dominated by a single fluid with a constant parameter γ_i. Key epochs of interest include the radiation fluid ($i = R$), where $p = \rho/3$ ($\gamma_R = 4/3$ or $w_R = 1/3$); incoherent matter ($i = M$), where $p = 0$ ($\gamma_M = 1$ or $w_M = 0$); and vacuum energy ($i = V$), where $p = -\rho$ ($\gamma_V = 0$ or $w_V = -1$), which is equivalent to a cosmological constant. Additionally, stiff matter fluid ($i = S$), characterized by $p = \rho$ ($\gamma_S = 2$ or $w_S = 1$), may also be relevant.

From Eq. (2.9), the density profile for each epoch is $\rho(t) \simeq \rho_i(t) \propto a(t)^{-3\gamma_i}$. Substituting this profile into the Friedmann equation (2.5) shows that for $\gamma_i > 2/3$ or $w_i > 1/3$, the curvature term, k^2/a^2, dominates only at later times, assuming a cosmological constant does not dominate earlier. Thus, for early Universe modeling, assuming a flat model ($k = 0$) is reasonable unless otherwise specified. This simplifies the Friedmann equation (2.5) and allows for integration, yielding the cosmological solutions

$$a(t) \propto t^{\frac{2}{3\gamma_i}}, \qquad H(t) = \frac{2}{3\gamma_i}\frac{1}{t}, \qquad \text{if } \gamma_i \neq 0, \tag{2.10}$$

$$a(t) \propto e^{\sqrt{\frac{\Lambda}{3}}t}, \qquad H(t) = \sqrt{\frac{\Lambda}{3}}, \qquad \text{if } \gamma_i = 0. \tag{2.11}$$

These solutions suggest that the early Universe was dominated by radiation, the intermediate Universe by matter, and, without vacuum energy, the late Universe would remain matter-dominated. However, current observations indicate otherwise, as the accelerated expansion of the Universe cannot be explained within the current framework with only a matter-dominated content [12, 13]. Furthermore, if the Universe underwent an initial period of inflation, there was a very early epoch dominated by vacuum energy, leading to an exponential expansion characterized by the cosmological solution (2.11).

Additionally, the Friedmann equation can be expressed in a more convenient form through the introduction of two dimensionless parameters: the critical density, determined by setting $\Lambda = k = 0$ in the aforementioned equation, defined as

$$\rho_c = \frac{3H^2(t)}{\kappa}, \tag{2.12}$$

and the dimensionless density parameter, denoted as $\Omega(t)$, representing the ratio of the energy density ρ to the critical density (ρ_c) at a given time

$$\Omega(t) \equiv \frac{\rho(t)}{\rho_c(t)}. \tag{2.13}$$

With these definitions, Eq. (2.5) can be reformulated as

$$\frac{k}{a^2H^2(t)} = \Omega(t) - 1. \tag{2.14}$$

This establishes a correlation between the sign of k and the sign of $\Omega - 1$. Specifically, for $k = 0$ (indicating a flat model), $\Omega = 1$; for $k = 1$ (indicating a closed model), $\Omega > 1$; and for $k = -1$ (indicating an (open model), $\Omega < 1$.

Using Eq. (2.9), and considering that the present-day value of the critical density parameter is given by $\rho_{c,0} = \frac{3H_0^2}{8\pi G}$, the density parameter as a function of redshift z can be written as

$$\Omega(z) = \frac{H_0^2}{H^2(z)}\left[\sum_i \Omega_{i,0}(1+z)^{3\gamma_i} + \Omega_\Lambda\right], \tag{2.15}$$

where $\Omega_\Lambda \equiv \frac{\Lambda}{3H_0^2}$ and $\Omega_{i,0} \equiv \frac{\rho_{i,0}}{\rho_{c,0}}$ represent the contributions from the cosmological constant and the i-th fluid component to the present-day density parameter, respectively.

Furthermore, the total density parameter can be expressed in terms of *partial density parameters* assigned to specific components or species i, such that $\Omega_0 = \sum_i \Omega_{i,0} = \sum \frac{\rho_{i,0}}{\rho_{c,0}}$, where $i = R$ denotes relativistic species and $i = M$ represents non-relativistic species. By integrating the energy conservation equation (2.7) using the barotropic equation (2.8), the Friedmann equation can ultimately be formulated as:

$$H^2(z) + \frac{k^2}{a^2(z)} = H_0^2 \left[\sum_i \Omega_{i,0}(1+z)^{3\gamma_i} + \Omega_\text{v} \right] . \tag{2.16}$$

This form of the Friedmann equation links the expansion rate of the Universe $H(z)$ with the contributions from various components, including matter, radiation, and vacuum energy, as well as the curvature of the Universe. The equation is fundamental for understanding the evolution of the Universe, particularly in predicting how different epochs, such as the radiation-dominated, matter-dominated, and vacuum energy-dominated eras, influence the overall dynamics and geometry of the cosmos.

2.2 Thermodynamics of the Primordial Universe

In addition to the previously discussed framework, studying the Primordial Universe requires a robust understanding of thermodynamics. This early stage of the Universe is deeply intertwined with statistical and dynamical processes that are fundamentally thermodynamic in nature, making thermodynamics a crucial pillar of the standard cosmological model during this period. The relationship between thermodynamics and gravitation, as well as its role in the primordial Universe, are extensive topics that could each warrant a dissertation on their own. Therefore, this thesis will focus on the essential aspects of thermodynamics necessary for a deeper understanding of the standard model of cosmology in the context of the Primordial Universe, particularly in what relates to baryogenesis.

2.2.1 Kinetic and Chemical Equilibrium

In thermodynamics, a system isolated from external influences will eventually reach a state of thermal equilibrium after sufficient time has passed. At this point, all observable properties—such as particle density (n), energy density (ρ), pressure (p), and entropy density (s)—stabilize into their most probable configurations. These macroscopic quantities can be expressed through integrals over the distribution function $f(x^a, p^a)$, which describes the system's phase space density. Given the Cosmological Principle, which asserts that the Universe is homogeneous and isotropic on large scales, it follows that the phase space distribution must also be isotropic and homogeneous. As a result, the distribution function simplifies to $f(x^a, p^a) = f(|\vec{\mathbf{p}}|, t) = f(E, t)$, where $E = \sqrt{\vec{\mathbf{p}}^2 + m^2}$ is the relativistic energy [96, 97]. Neglecting explicit time dependence (later revealed through its link to temperature), the phase space distribution for particle species i in kinetic equilibrium—under the assumption of an ideal gas—takes the form of either the Fermi-Dirac (FD) or Bose-Einstein (BE) distributions [96, 97]:

$$f_i(\vec{p}) = \left[\exp\left(\frac{E_i(\vec{p}) - \mu_i}{T} \right) \pm 1 \right]^{-1} , \tag{2.17}$$

where E_i is the energy of species i, and m_i is the rest mass. The term μ_i is the chemical potential, with the plus sign indicating fermions (FD statistics) and the minus sign indicating bosons (BE statistics). If the ± 1 term is omitted, the result approximates the Maxwell-Boltzmann (MB) distribution for classical and distinguishable particles. While this classical approximation is not exact, it remains useful in the absence of degenerate Fermi species (where $\mu_i \gtrsim T_i$) or Bose condensation. In such cases, the deviation from FD or BE statistics is typically minimal, often less than 10% [98]. This approximation becomes particularly effective for non-relativistic particles where $m_i \gg T_i$ and $m_i \gg T + \mu_i$, in which case the MB distribution becomes essentially accurate.

To expand on the concept, it is necessary to consider the role of the chemical potential, a key thermodynamic variable in systems with variable particle numbers. The chemical potential represents the infinitesimal change in energy due to the addition of one particle of a given type. It can be understood through the fundamental thermodynamic relation [96]:

$$dE = TdS - pdV + \sum_i \mu_i dN_i, \tag{2.18}$$

where S is entropy, V is volume, and N_i is the number of particles of species i. In equilibrium gases, the interaction term $\sum_i \mu_i dN_i = 0$ reflects the conservation of chemical potentials. A deviation from this condition would change the particle numbers of the species involved, ultimately lowering the system's free energy, $F = E - TS$, where E is internal energy. Under constant temperature and volume, this relation simplifies to:

$$dF = \sum_i \mu_i dN_i. \tag{2.19}$$

For equilibrium to hold, both kinetic and chemical equilibrium must be maintained. In equilibrium, the distribution functions not only take the familiar thermal forms from Eq. (2.17), but the chemical potentials of interacting species are also interconnected. In chemical equilibrium, the chemical potentials of species participating in reactions are conserved. For example, in a reaction like $a_1 + a_2 + \cdots \leftrightarrow b_1 + b_2 + \ldots$, the chemical potentials follow the rule:

$$\sum_k \mu_{a_k} = \sum_k \mu_{b_k}. \tag{2.20}$$

This principle also applies to radiation. Since photons can be emitted or absorbed in arbitrary reactions, any reaction involving charged particles, such as $i + i \to i + i + \gamma$, implies that $\mu_\gamma = 0$ in equilibrium. In reactions involving particle-antiparticle annihilation, such as $i + \bar{i} \leftrightarrow 2\gamma$, equilibrium requires that:

$$\mu_i + \mu_{\bar{i}} = 0, \tag{2.21}$$

indicating that particle and antiparticle chemical potentials are equal in magnitude but opposite in sign. For self-conjugate particles (where $i = \bar{i}$) or in cases of symmetry between particles and antiparticles ($n_i = n_{\bar{i}}$), chemical equilibrium demands that $\mu_i = 0$. Thus, the distribution function in equilibrium depends solely on temperature, reducing the phase space description to $f(T)$.

2.2.2 Free Particle Gases and Interactions in an Expanding Universe

In the context of an expanding Universe, it is essential to apply equilibrium thermodynamics with caution. The dynamic nature of such a Universe implies that temperature (T) and chemical potential (μ) are not static but evolve to ensure the conservation of energy and particle number. An expanding Universe represents a non-equilibrium system, causing deviations from standard equilibrium distribution functions and necessitating explicit consideration of time-dependent behaviors.

Consider gases composed of stable, non-interacting particles—particles that neither decay nor engage significantly with their environment. For these freely propagating particles, the number of particles in a given volume $\mathrm{d}^3\mathbf{x}$ within the momentum interval $\mathrm{d}^3\mathbf{p}$ is conserved [96, 97], and can be represented as

$$dN_i = \frac{g_i}{(2\pi)^3} f_i(\mathbf{x},\, \mathbf{p},\, t)\, \mathrm{d}^3\mathbf{x}\mathrm{d}^3\mathbf{p} = \mathrm{Cte}\,, \tag{2.22}$$

where g_i denotes the internal degrees of freedom (e.g., spin states) of particle i [96]. According to the SCM, gases of freely moving particles exhibit homogeneity and isotropy, implying that their distribution functions are spatially uniform and depend solely on momenta and time. Furthermore, the physical three-momentum decreases with the scale factor, following ($|\mathbf{p}| \propto a^{-1}$), while the proper volume spatial element scales as ($d^3\mathbf{x} \propto a^3$). By examining Eq. (2.22), one can infer that if the distribution function at a specific time ($t = t_d$) is known, such that $f_i(|\mathbf{p}_d|, t_d) \equiv f_{id}(|\mathbf{p}_d|)$, then at a later time ($t > t_d$), the distribution function adheres to the relation $f_i(|\mathbf{p}|,t) d^3\mathbf{x}\mathrm{d}^3\mathbf{p} = f_{id}(|\mathbf{p}_d|)\mathrm{d}^3\mathbf{x}_d\mathrm{d}^3\mathbf{p}_d = f_{id}(a|\mathbf{p}|/a_d) d^3\mathbf{x}\mathrm{d}^3\mathbf{p}$. This indicates that the distribution function is determined by the redshifted momentum. Thus, for a stable particle species in equilibrium that decouples at ($t = t_d$), its distribution function before decoupling follows the usual thermal form, while after decoupling, it simplifies to $f_i^{eq}(a|\mathbf{p}|/a_d)$.

When considering interactions, it is crucial to assess whether particles are coupled or decoupled by comparing the interaction rate, Γ_{int}, to the Universe's expansion rate

$$\Gamma_{\mathrm{int}} > H, \qquad \text{coupled}\,, \tag{2.23}$$

$$\Gamma_{\mathrm{int}} < H, \qquad \text{decoupled}\,. \tag{2.24}$$

Although true equilibrium is challenging to achieve in an expanding Universe, the gradual expansion often allows particle distributions to approximate local equilibrium. Given the homogeneity of the Universe, local thermodynamic quantities reflect global values. Therefore, when particle interactions are significantly faster than the expansion rate, equilibrium-like distributions can emerge on the timescale of expansion. Particles will approach equilibrium-like states whenever condition (2.23) is satisfied. However, when $\Gamma_{\mathrm{int}} < H$, equilibrium does not necessarily break down. For this to occur, the rate of a crucial reaction maintaining equilibrium must remain below the Hubble parameter H.

For a stable and massless particle species i with $\mu_i = 0$ that is in equilibrium at $t < t_d$ and decouples at t_d, its distribution function at later times is given by

$$f_i(|\mathbf{p}|,\, t) = f_i^{eq}\left(\frac{a(t)|\mathbf{p}(t)|}{a_d}\right) = \left[\exp\left(\frac{|\mathbf{p}(t)|a(t)}{T_d a_d}\right) \pm 1\right]^{-1} = f_i^{eq}\left(\frac{|\mathbf{p}|}{T_i}\right)\,. \tag{2.25}$$

Here, $T_d = T(t_d)$ and $a_d = a(t_d)$ denote the temperature and scale factor at decoupling, respectively. The temperature of the decoupled species at any subsequent time t is:

$$T_i(t) = \frac{a_d}{a(t)} T_d\,. \tag{2.26}$$

Although the decoupled particle species may not be in thermal equilibrium, its distribution function retains the same shape as the equilibrium distribution function for massless particles. However, the effective temperature continually decreases as $T_i \propto a^{-1}$. For observed decoupled photons of the Cosmic Microwave Background with negligible chemical potential ($|\mu_\gamma/T_\gamma| < 10^{-4}$) [99], if the Universe was ever in equilibrium, the photon distribution has consistently been Planckian (as given by Eq. (2.25) with the $-$ sign). Thus, the photon number density, energy density, and pressure can be computed as

$$n_\gamma = \frac{g_\gamma}{(2\pi)^3}\int f_\gamma^{Pl}(|\mathbf{p}|)\mathrm{d}^3\mathbf{p} = \frac{g_\gamma}{2\pi^2}\int \frac{E_\gamma^2}{e^{E_\gamma/T_\gamma}-1}\mathrm{d}E_\gamma = \frac{2\zeta(3)}{\pi^2}T_\gamma^3\,, \tag{2.27}$$

$$\rho_\gamma = \frac{g_\gamma}{(2\pi)^3}\int E_\gamma f_\gamma^{Pl}(|\mathbf{p}|)\mathrm{d}^3\mathbf{p} = \frac{g_\gamma}{2\pi^2}\int \frac{E_\gamma^3}{e^{E_\gamma/T_\gamma}-1}\mathrm{d}E_\gamma = \frac{\pi^2}{15}T_\gamma^3\,, \tag{2.28}$$

$$p_\gamma = \frac{g_\gamma}{(2\pi)^3}\int \frac{|\vec{\mathbf{p}}|^2}{3E_\gamma} f_\gamma^{Pl}(|\mathbf{p}|)\mathrm{d}^3\mathbf{p} = \frac{g_\gamma}{6\pi^2}\int \frac{E_\gamma^3}{e^{E_\gamma/T_\gamma}-1}\mathrm{d}E_\gamma = \frac{1}{3}\rho_\gamma^{eq} = \frac{\pi^2}{45}T_\gamma^3\,, \tag{2.29}$$

where $g_\gamma = 2$ accounts for the two photon polarization states, and the integration over all angles was performed. For other potentially decoupled particle species, their number density at any time is given by

$$n_i = \frac{g_i}{(2\pi)^3}\int\left[\exp\left(\frac{|\mathbf{p}|a}{T_d a_d}\right)\pm 1\right]^{-1}\mathrm{d}^3\mathbf{p} = g^n_{\mathrm{eff}_i}\left(\frac{\zeta(3)T_\mathrm{d}^3}{\pi^2}\right)\left(\frac{a_d}{a}\right)^3\,, \tag{2.30}$$

where $g^n_{\mathrm{eff}_i} = g_{\mathrm{eff}_i} = g_i$ for bosons or $g^n_{\mathrm{eff}_i} = 3/4 g_i$ for fermions. If these particle species were in equilibrium with photons prior to their decoupling, their number density remains comparable to that of photons. These decoupled species thus persist as relic backgrounds in the Universe. The temperature at which decoupling occurs is commonly referred to as the "freezing temperature,"denoted T_f. This temperature can be approximately estimated using the "freezing relation":

$$\Gamma_{\mathrm{int}}(T_f) = H(T_f)\,. \tag{2.31}$$

In cases where a particle species i decouples at a time t_d when it has transitioned to a non-relativistic state ($T_d \ll m_i$), and when $m_i - \mu_i \gg T$, its distribution function follows the Maxwell-Boltzmann (MB) distribution at the time of decoupling. Here, the kinetic energy is much smaller than the rest mass m_i, allowing the approximation $E_i = m_i + p^2/(2m_i)$. For such particles, the distribution function at later times $(t > t_d)$ is

$$f_i(|\vec{\mathbf{p}}|,t) = f_i^{MB}\left(\frac{a(t)}{a}p(t)\right) = \frac{1}{(2\pi)^3}\exp\left(-\frac{m_i-\mu_{iD}}{T_d}\right)\exp\left(\frac{|\vec{\mathbf{p}}|}{2m_i^2}\frac{a(t)^2}{a_d^2 T_d^2}\right)\,, \tag{2.32}$$

where μ_{iD} is the chemical potential at the time of decoupling. Thus, post-decoupling, the distribution function retains its equilibrium form, albeit with an effective chemical potential $\mu_i(t)$ and temperature T_i given by

$$\mu_i(t) = m_i + \left(\frac{\mu_{iD}-m_i}{T_d}\right)T_i(t)\,, \qquad T_i(t) = \left(\frac{a_d}{a(t)}\right)^2 T_d\,. \tag{2.33}$$

This results in an effective temperature that decreases more rapidly than for decoupled massless particle species. Particles that decouple in a non-relativistic state are often considered candidates for "cold dark matter,"as they remain as a cold relic background in the Universe.

If a particle species i has a small but non-zero mass and is relativistic at the time of decoupling ($m_i \ll T_d$), its distribution function becomes ”frozen” in the form characteristic of massless particles. The spectrum remains thermal with a temperature that decreases with the scale factor a^{-1} as long as $T \gg m_i$. Once the temperature of the thermal bath falls below the particle's mass, the distribution function and number density adopt a form consistent with relativistic particles. Although the distribution function transitions to the MB distribution form, the energy density aligns with that of a non-relativistic particle species, i.e., $\rho \simeq mn$. As a result, the equilibrium distribution function is no longer maintained, characterized by $T \propto a^{-1}$. This scenario is associated with "hot dark matter"and "warm dark matter"[100, 101, 102, 103], where particles decouple in a relativistic state but maintain massless distribution functions in momentum space.

2.2.3 The Matter Content of the Universe

When the primary components of the Universe reach equilibrium, it becomes possible to accurately estimate key thermodynamic quantities such as the total number density, energy density, and pressure by considering only the contributions from species in equilibrium. In these scenarios, the calculations for these quantities are straightforward, as outlined earlier.

Even if the Universe had a past equilibrium state, it is reasonable to assume that, in many instances, even when equilibrium between the major components is disrupted, the matter composition can still be effectively described. This can be done by incorporating contributions from particle species that follow thermal distribution functions, albeit with temperatures distinct from the equilibrium temperature of the cosmic medium, denoted by T. Including these contributions into the overall equilibrium quantities is not only advantageous but also relatively simple. Hence, if the non-equilibrium components can be represented by an equilibrium distribution function, the total number density, energy density, and pressure can be expressed as follows

$$\begin{aligned} n = &\sum_i \frac{g_i}{(2\pi)^3}\int f_i(\vec{\mathbf{p}})\,\mathrm{d}^3p = \sum_i \frac{g_i}{2\pi^2}\int_{m_i}^{\infty} \frac{\sqrt{E_i^2-m_i^2}E_i}{\exp[(E_i-\mu_i)/T_i]\pm 1}\,\mathrm{d}E_i \\ &= \frac{T^3}{2\pi^2}\mathcal{N}_*\left(\left\{\frac{T_i}{T}\right\},\left\{\frac{m_i}{T_i}\right\},\left\{\frac{\mu_i}{T_i}\right\}\right), \end{aligned} \tag{2.34}$$

$$\begin{aligned} \rho = &\sum_i \frac{g_i}{(2\pi)^3}\int E_i(\vec{\mathbf{p}})f_i(\vec{\mathbf{p}})\,\mathrm{d}^3p = \sum_i \frac{g_i}{2\pi^2}\int_{m_i}^{\infty} \frac{\sqrt{E_i^2-m_i^2}E_i^2}{\exp[(E_i-\mu_i)/T_i]\pm 1}\,\mathrm{d}E_i \\ &= \frac{\pi^2T^4}{30}\mathcal{E}_*\left(\left\{\frac{T_i}{T}\right\},\left\{\frac{m_i}{T_i}\right\},\left\{\frac{\mu_i}{T_i}\right\}\right), \end{aligned} \tag{2.35}$$

$$\begin{aligned} p = &\sum_i \frac{g_i}{(2\pi)^3}\int \frac{|\vec{\mathbf{p}}|^2 f_i(\vec{\mathbf{p}})}{3E_i(\vec{\mathbf{p}})}\,\mathrm{d}^3p = \sum_i \frac{g_i}{6\pi^2}\int_{m_i}^{\infty} \frac{(E_i^2-m_i^2)^{3/2}}{\exp[(E_i-\mu_i)/T_i]\pm 1}\,\mathrm{d}E_i \\ &= \frac{\pi^2T^4}{90}\mathcal{P}_*\left(\left\{\frac{T_i}{T}\right\},\left\{\frac{m_i}{T_i}\right\},\left\{\frac{\mu_i}{T_i}\right\}\right), \end{aligned} \tag{2.36}$$

where the second relation follows from the angular integration, using $E\mathrm{d}E = |\vec{\mathbf{p}}|\,\mathrm{d}|\vec{\mathbf{p}}|$. The terms $\mathcal{E}_*(\{x_i\},\ \{z_i\},\ \{y_i\}) = \sum_i \mathcal{E}_i^{\pm}(x_i,\ z_i,\ y_i)$, $\mathcal{N}_*(\{x_i\},\ \{z_i\},\ \{y_i\}) = \sum_i \mathcal{N}_i^{\pm}(x_i,\ z_i,\ y_i)$, and $\mathcal{P}_*(\{x_i\}, \{z_i\}, \{y_i\}) = \sum_i \mathcal{P}_i^{\pm}(x_i, z_i, y_i)$ serve as a convenient parametrization of the *effective degrees of freedom* in the number density, energy density, and pressure for a genuine Bose-Einstein gas in thermal equilibrium, namely, $\rho = \mathcal{E}_*\rho_\gamma/g_\gamma$, $n = \mathcal{N}_* n_\gamma/\zeta(3)g_\gamma$, and $p = \mathcal{P}_* p_\gamma/g_\gamma$. Here,

$$\mathcal{N}_i^\pm\left(\frac{T_i}{T},\, z_i = \frac{m_i}{T_i},\, y_i = \frac{\mu_i}{T_i}\right) \equiv g_i\left(\frac{T_i}{T}\right)^3 \int_{z_i}^{\infty} \frac{\sqrt{u^2 - z_i^2}\,u}{\exp(u-y_i)\pm 1}\,\mathrm{d}u\,, \tag{2.37}$$

$$\mathcal{E}_i^\pm\left(\frac{T_i}{T},\, z_i = \frac{m_i}{T_i},\, y_i = \frac{\mu_i}{T_i}\right) \equiv \frac{15}{\pi^4} g_i\left(\frac{T_i}{T}\right)^4 \int_{z_i}^{\infty} \frac{\sqrt{u^2 - z_i^2}\,u^2}{\exp(u-y_i)\pm 1}\,\mathrm{d}u\,, \tag{2.38}$$

$$\mathcal{P}_i^\pm\left(\frac{T_i}{T},\, z_i = \frac{m_i}{T_i},\, y_i = \frac{\mu_i}{T_i}\right) \equiv \frac{15}{\pi^4} g_i\left(\frac{T_i}{T}\right)^4 \int_{z_i}^{\infty} \frac{(u^2 - z_i^2)^{3/2}}{\exp(u-y_i)\pm 1}\,\mathrm{d}u\,, \tag{2.39}$$

where $u = E/T$. These expressions encapsulate the individual contributions of each species to the total degrees of freedom across the thermodynamic quantities.

The statistical framework presented here connects the primary thermodynamic variables, the number density, the energy density, and the pressure, with the temperature of the surrounding medium. All relevant quantities are expressed in terms of the photon temperature, which serves as the equilibrium temperature of the medium. The parameters $\mathcal{N}*, \mathcal{E}*, \mathcal{P}_*$ were introduced to simplify the analysis, as they encapsulate the key behaviors of each thermodynamic variable. Additionally, using temperature, mass, and chemical potential as parameters facilitates the computation of the required integrals, providing a useful basis for various approximations, such as $m \ll T$, applicable in the ultra-relativistic limit. While integrals such as (2.37)–(2.39) are often not expressible in terms of elementary functions, they can be solved numerically or, in some cases, analytically under specific conditions.

2.2.3.1 Non-Relativistic Case

In the case where Maxwell-Boltzmann statistics are approximately valid, the integrals in equations (2.37-2.39) can be computed and expressed in terms of special functions. Specifically, these integrals take the following form

$$\mathcal{N}_i^{\mathrm{MB}}\left(\frac{T_i}{T}, \frac{m_i}{T_i}, \frac{\mu_i}{T_i}\right) = \frac{\pi^4}{45}\frac{T}{T_i}\mathcal{P}_i^{\mathrm{MB}}\left(\frac{T_i}{T}, \frac{m_i}{T_i}, \frac{\mu_i}{T_i}\right) = g_i\left(\frac{T_i}{T}\right)^3\left(\frac{m_i}{T_i}\right)^2 e^{\mu_i/T_i} K_2(z_i), \tag{2.40}$$

$$\mathcal{E}_i^{\mathrm{MB}}\left(\frac{T_i}{T}, \frac{m_i}{T_i}, \frac{\mu_i}{T_i}\right) = \frac{45}{\pi^4}\left(\frac{T_i}{T}\right)\left(1 + \frac{K_1(z_i)}{3K_2(z_i)}\right)\mathcal{N}_i^{\mathrm{MB}}. \tag{2.41}$$

Here, $K_n(z)$ represents a modified Bessel function of the second kind, and the superscript refers to the interpretation of the integrals in terms of Maxwell-Boltzmann (MB) distribution functions, which exclude the ± 1 terms present in the original functions. As previously mentioned, in situations where neither degenerate fermions nor a Bose condensate are present, this approximation introduces only a small quantitative difference from the exact Fermi-Dirac (FD) and Bose-Einstein (BE) statistics. As a result, under the physical conditions where particles are non-relativistic ($m_i \gg T_i$) and $m_i \gg T_i + \mu_i$, this approximation becomes highly accurate. This second condition leads to occupation numbers significantly below unity, indicating a dilute gas, a scenario consistent with earlier assumptions. Such conditions are commonly met in cosmological contexts, although they are violated in high-density environments such as white dwarfs and neutron stars. Consequently, quantities such as $\mathcal{N}_i^j$, $\mathcal{E}_i^j$, and $\mathcal{P}_i^j$ become independent of the statistical framework (with $j = \mathrm{MB}, +, -$).

For large z values ($m_i \gg T$), the approximation $K_2(z_i) = \sqrt{\pi/(2z_i)}e^{-z} + O(1/z_i)$ and $\left(1 + \frac{K_1(z_i)}{3K_2(z_i)}\right) = \frac{1}{2} + \frac{z_i}{3}$ leads to the following expressions

$$\mathcal{N}_i^{\pm}\left(\frac{T_i}{T},\frac{m_i}{T_i},\frac{\mu_i}{T_i}\right) = g_i\sqrt{\frac{\pi}{2}}\left(\frac{T_i}{T}\right)^3\left(\frac{m_i}{T_i}\right)^{\frac{3}{2}} e^{-\frac{m_i-\mu_i}{T_i}}, \tag{2.42}$$

$$\mathcal{P}_i^{\pm}\left(\frac{T_i}{T},\frac{m_i}{T_i},\frac{\mu_i}{T_i}\right) = \frac{45}{\pi^4}\left(\frac{T_i}{T}\right)\mathcal{N}_i^{\pm}\left(\frac{T_i}{T},\frac{m_i}{T_i},\frac{\mu_i}{T_i}\right), \tag{2.43}$$

$$\mathcal{E}_i^{\pm}\left(\frac{T_i}{T},\frac{m_i}{T_i},\frac{\mu_i}{T_i}\right) = \frac{45}{\pi^4}\left(\frac{T_i}{T}\right)\left[\frac{1}{2}+\left(\frac{m_i}{3T_i}\right)\right]\mathcal{N}_i^{\pm}\left(\frac{T_i}{T},\frac{m_i}{T_i},\frac{\mu_i}{T_i}\right). \tag{2.44}$$

This yields the non-relativistic number density (n_i), energy density (ρ_i), and pressure (p_i) as

$$n_i = g_i\left(\frac{m_iT_i}{2\pi}\right)^{3/2} e^{-\frac{m_i-\mu_i}{T_i}}, \tag{2.45}$$

$$\rho_i = m_in_i + \frac{3}{2}n_iT_i, \tag{2.46}$$

$$p_i = n_iT_i \ll \rho_i. \tag{2.47}$$

2.2.3.2 Relativistic Case

In the relativistic limit where $T_i \gg m_i$ and the chemical potential is approximately zero ($\mu_i = 0$), it is possible to derive the corresponding expressions by simplifying the earlier equations. Under these conditions, the particle species are relativistic, and the chemical potential can be reasonably neglected, leading to

$$\mathcal{N}_i^{\pm}\left(\frac{T_i}{T},0,0\right) = 2\zeta(3)g_{\text{eff}_i}\left(\frac{T_i}{T}\right)^3, \tag{2.48}$$

$$\mathcal{E}_i^{\pm}\left(\frac{T_i}{T},0,0\right) = \mathcal{P}_i^{\pm}\left(\frac{T_i}{T},0,0\right) = g_{\text{eff}_i}\left(\frac{T_i}{T}\right)^4. \tag{2.49}$$

This results in the relativistic number density and energy density for species i as

$$n_i = \frac{\zeta(3)}{\pi^2}g^n_{\text{eff}_i}T_i^3, \tag{2.50}$$

$$\rho_i = \frac{\pi^2}{30}g_{\text{eff}_i}T_i^4 = 3p_i, \tag{2.51}$$

where $g^n_{\text{eff}_i} = \frac{3}{4}g_i$ and $g_{\text{eff}_i} = \frac{7}{8}g_i$ for fermions, and $g^n_{\text{eff}_i} = g_{\text{eff}_i} = g_i$ for bosons.

2.2.3.3 Total Energy Density

The total energy density in a system with both relativistic and non-relativistic particles can be approximated by primarily considering the relativistic species, as their contribution to pressure and energy density dominates. This can be expressed as[96]

$$\rho = \frac{\pi^2}{30}g_*T^4, \tag{2.52}$$

where the effective degrees of freedom are summed over as

$$g_*(T) = \sum_{\text{bosons}} g_i \left(\frac{T_i}{T}\right)^4 + \frac{7}{8} \sum_{\text{fermions}} g_i \left(\frac{T_i}{T}\right)^4 . \tag{2.53}$$

This sum separates into contributions from species in thermal equilibrium ($T_i = T$) and those decoupled from the photon gas ($T_i \neq T$)

$$g_*^{\text{equilibrium}} = \sum_{\text{bosons}} g_i + \frac{7}{8} \sum_{\text{fermions}} g_i , \tag{2.54}$$

$$g_*^{\text{decoupled}}(T) = \sum_{\text{bosons}} g_i \left(\frac{T_i}{T}\right)^4 + \frac{7}{8} \sum_{\text{fermions}} g_i \left(\frac{T_i}{T}\right)^4 . \tag{2.55}$$

2.2.3.4 Net Particle Number

The comparison between a particle species and its corresponding antiparticle is often of interest, especially when calculating the net particle excess in a state of full equilibrium. In chemical equilibrium, the chemical potential of a particle species i^+ and its antiparticle i^- are equal in magnitude but opposite in sign, represented as $\mu \equiv \mu_{i^+} = -\mu_{i^-}$. Under this condition, the net number density of particles i^+ relative to antiparticles i^- can be determined using Eq. (2.34), leading to the following expression [96]

$$n_{i^+} - n_{i^-} = \begin{cases} \frac{g_i T_i^3}{6\pi^2} \left[\pi^2 \left(\frac{\mu}{T_i}\right) + \left(\frac{\mu}{T_i}\right)^3 \right], & \text{for relativistic fermions} \, (T_i \gg m_i) \\ \frac{g_i T_i^3}{6\pi^2} \left[2\pi^2 \left(\frac{\mu}{T_i}\right) - \frac{1}{3} \left(\frac{\mu}{T_i}\right)^3 \right], & \text{for relativistic bosons} \, (T_i \gg m_i) \\ 2 g_i \left(\frac{m_i T_i}{2\pi}\right)^{3/2} \sinh\left(\frac{\mu}{T_i}\right) e^{\left(-\frac{m_i}{T_i}\right)}, & \text{for all non-relativistic species} \, (T_i \ll m_i) \end{cases} \tag{2.56}$$

For practical purposes, it is often helpful to express these quantities in terms of small chemical potentials, particularly in cases where $|\mu| < m$ (where no Bose-Einstein condensation occurs). In this regime, the net particle number is given by

$$n_{i^+} - n_{i^-} = \frac{g_i a^{\pm c}}{6} T_i^3 \left(\frac{\mu_i}{T_i}\right) \alpha_i^{\pm c} \left(\frac{m_i}{T_i}\right) , \tag{2.57}$$

where

$$\alpha_i^{\pm c} \left(z_i = \frac{m_i}{T_i} \right) \equiv \frac{6}{\pi^2 a^{\pm c}} \int_{z_i}^{\infty} u \sqrt{u^2 - z_i^2} \frac{e^u}{(e^u \pm c)^2} \, \mathrm{d}u , \qquad (u = E_i/T) , \tag{2.58}$$

with $a^{+1} = 1$, $a^{-1} = a^{\pm 0} = 2$. The superscripts $+1$, -1, and ± 0 correspond to Fermi-Dirac, Bose-Einstein, and Maxwell-Boltzmann statistics, respectively. In the massless limit ($m_i = 0$), the function $\alpha^{\pm c}(0)$ simplifies to $\alpha^{\pm c}(0) = 1$.

2.2.4 Entropy in the Expanding Universe

Entropy holds a crucial position in the thermodynamic description of the Universe, particularly due to its relationship with the scale factor. Within the field of thermodynamics, entropy is also fundamental to the discipline's core principles. This is especially true in scenarios involving a varying number of particles, where entropy's significance is highlighted by the general formulation given in Eq. (2.18). This formulation is structured around the understanding that energy and the number of particles are extensive properties, scaling proportionally with the volume of the system, whereas temperature and pressure manifest as local characteristics independent of volume. Consequently, entropy itself is classified as an extensive property. It is beneficial, therefore, to reformulate the fundamental thermodynamic equation by expressing energy, number of particle, and entropy in terms of their densities within a cosmological volume V. This reformulation leads to the following expression

$$(Ts - \rho - p + \mu n)dV + (Tds - d\rho + \mu dn)V = 0\,, \tag{2.59}$$

where $\rho = E/V$, $n = N/V$ and $s = S/V$. This relation is valid both for the entire system and any of its parts and so, using it for a region of constant volume inside the system it is possible to obtain $Tds = d\rho - \mu dn$ and using it subsequently for the entire system, gives the entropy density [104]

$$s = \sum_i \frac{\rho_i + p_i - \sum_i \mu_i n_i}{T_i} = \frac{2\pi^2}{45}\mathcal{S}_*\left(\left\{\frac{T_i}{T}\right\}, \left\{\frac{m_i}{T_i}\right\}, \left\{\frac{\mu_i}{T_i}\right\}\right) T^3\,, \tag{2.60}$$

where $S_*(\{T_i/T\}, \{m_i/T\}, \{\mu_i/T\}) = \sum_i S_i^{\pm}(T_i/T, m_i/T, \mu_i/T)$ with $S_i^{\pm}$ defined as

$$S_i^{\pm}\left(\frac{T_i}{T}, \frac{m_i}{T_i}, \frac{\mu_i}{T_i}\right) \equiv \frac{T}{T_i}\left(\frac{3}{4}\mathcal{E}_i^{\pm} + \frac{1}{4}\mathcal{P}_i^{\pm}\right) - \frac{45}{4\pi^4}\frac{\mu_i}{T_i}\mathcal{N}_i^{\pm}\,, \tag{2.61}$$

represents the contributions of each species i to the effective degrees of freedom within entropy. Equation (2.60) corresponds to the general expression without assuming any specific case, where the computation of such a general case requires numerical methods. However, the relativist and non-relativist cases can be calculated analytically.

In the relativistic case, considering $T_i \gg m_i$ and vanishing chemical potentials, the expression for $\mathcal{S}_i^{\pm}$ is given by

$$\mathcal{S}_i^{\pm}\left(\frac{T_i}{T}, 0, 0\right) = \frac{g_{\text{eff}_i}}{2\zeta(3)g^n_{\text{eff}_i}}\mathcal{N}_i^{\pm}\left(\frac{T_i}{T}, 0, 0\right) = g_{\text{eff}_i}\left(\frac{T_i}{T}\right)^3\,, \tag{2.62}$$

which in turn allows to compute the total energy density for relativistic species

$$s_{relativistic} = \sum_i \frac{2\pi^2}{45} g_{\text{eff}_i} T_i^3\,. \tag{2.63}$$

Another way to obtain this result is to use directly the first equality of Eq. (2.60) with $\mu = 0$ and considering that in the relativistic scenario, the energy density and pressure have the relation $\rho = 3p$, allowing in combination with Eq. (2.52) to write the entropy density for relativistic species as

$$s_{relativistic} = \sum_i \frac{\rho_i + p_i}{T_i} = \frac{4}{3}\sum_i \frac{\rho_i}{T_i} = \sum_i \frac{2\pi^2}{45} g_{\text{eff}_i} T_i^3\,. \tag{2.64}$$

For the non-relativistic case, one considers $m_i \gg T_i$ satisfying the condition $m_i - \mu_i \gg T$ that allows to compute $\mathcal{S}_i^{\pm}$ as

$$\mathcal{S}_i^{\pm}\left(\frac{T_i}{T}, \frac{m_i}{T_i}, \frac{\mu_i}{T_i}\right) = \frac{45 g_i}{4\pi^4}\sqrt{\frac{\pi}{2}}\left(\frac{5}{2} + \frac{m_i - \mu_i}{T_i}\right)\left(\frac{T_i}{T}\right)^3\left(\frac{m_i}{T_i}\right)^{\frac{3}{2}} e^{\frac{\mu_i - m_i}{T_i}}\,, \tag{2.65}$$

leading to the following total entropy density for non-relativistic species

$$s_{non-relativistic} = \sum_i n_i \left[\frac{5}{2} + \ln\left(\frac{g_i}{n_i}(\frac{m_i T_i}{2\pi})^{\frac{3}{2}}\right)\right] , \tag{2.66}$$

where Eq. (2.45) was used to express the entropy density in terms of the number density.

Once more, this result can be obtained directly by using the first equality of Eq. (2.60), Eq. (2.46) and Eq. (2.47), yielding [104]

$$s_{non-relativistic} = \sum_i \frac{5}{2} n_i + \frac{m_i - \mu_i}{T} n_i . \tag{2.67}$$

To calculate the total entropy density, one can approximate that relativistic species will dominate the contribution when comparing the results for relativistic and non-relativistic cases. Therefore, using Eq.(2.52), the total entropy density can be expressed as[96]

$$s = \sum_i \frac{\rho_i + p_i}{T_i} = \frac{2\pi^2}{45} g_{*S} T^3 , \tag{2.68}$$

where

$$g_{*S} = \sum_{i=\text{bosons}} g_i \left(\frac{T_i}{T}\right)^3 + \frac{7}{8} \sum_{i=\text{fermions}} g_i \left(\frac{T_i}{T}\right)^3 . \tag{2.69}$$

A notable point to consider is that when all relativistic species are in thermal equilibrium, that is, they share the same temperature, it is a good approximation to assume that g_{*S} equals g_* [96]. The entropy of all relativistic species remains conserved as long as their distribution functions stay thermal. In this scenario, any entropy production from non-equilibrium processes is negligible compared to the total entropy, which is overwhelmingly dominated by the relativistic species. Therefore, treating the expansion of the Universe as adiabatic is an excellent approximation. In this context, entropy serves as a reliable tool for tracking the evolution of the scale factor in relation to temperature, which is then given by the following expression

$$a \propto g_{*S}^{-1/3}(T)\, T^{-1} . \tag{2.70}$$

Finally, the second law of thermodynamics plays a central role in shaping our understanding of the early Universe. According to this law, the entropy of any closed system must increase, and it only remains constant during equilibrium or adiabatic processes. In an expanding Universe, applying the fundamental principles of thermodynamics to a comoving volume $V = a^3$ gives the following differential equation, in the case of thermal equilibrium

$$\frac{d(a^3 s)}{dt} = 0 . \tag{2.71}$$

This equation reveals that energy conservation can be interpreted directly in terms of entropy. When the chemical potentials vanish, the above equation describes the conservation of entropy in a comoving volume, $S = a^3 s$. The discussion concludes with two key points. First, for a Universe undergoing adiabatic expansion, a direct relationship exists between its expansion (or redshift) and its cooling, given by

$$a\left(T,\left\{\frac{T_i}{T}\right\},\left\{\frac{m_i}{T_i}\right\},\left\{\frac{\mu_i}{T_i}\right\}\right)=cte\left(\frac{45}{2\pi^2}\right)^{1/3}\mathcal{S}_*^{-1/3}\left(\left\{\frac{T_i}{T}\right\},\left\{\frac{m_i}{T_i}\right\},\left\{\frac{\mu_i}{T_i}\right\}\right)T^{-1}, \tag{2.72}$$

$$(1+z_1)\,T_0=\left(\frac{\mathcal{S}_*^{1/3}(\{T_i/T_1\},\{m_i/T_i\},\{\mu_i/T_i\})}{\mathcal{S}_*^{1/3}(\{T_i/T_0\},\{m_i/T_i\},\{\mu_i/T_i\})}\right)T_1\,, \tag{2.73}$$

and the second is related to the number of particles. Considering a number of a given species i in comoving volume, $V_i=a^3n_i$ is proportional to the number density of the species N divided by s, that is, $V_i=cte.\times n_i/s=cte\times N$ where N is conveniently defined as

$$N\equiv\frac{n_i}{s}. \tag{2.74}$$

Subsequently, from Eq. (2.72) it is possible to establish the differential relation

$$\frac{da}{a}=H\mathrm{d}t=-\left(\frac{\mathrm{d}\mathcal{S}_*}{3\mathcal{S}_*}+\frac{dT}{T}\right)\quad\Rightarrow\quad H=-\left(\frac{\dot{\mathcal{S}}_*}{3\mathcal{S}_*}-\frac{\dot{T}}{T}\right), \tag{2.75}$$

which in turn, combined with the dynamical Eq. (2.5) for the flat model, written in terms of $\rho=\pi^2\mathcal{E}_*T^4/30$ can be used to find the *time-temperature relation*

$$t=-\int\left(\frac{8\pi^3G_N}{90}\mathcal{E}_*T^4\right)^{-1/2}\left(\frac{\mathrm{d}\mathcal{S}_*}{3\mathcal{S}_*}+\frac{dT}{T}\right). \tag{2.76}$$

which relates the age of the Universe with the temperature.

2.2.5 Baryons in the early Universe

As seen in the previous section, it becomes clear that the conservation of entropy within a comoving volume can be utilized to establish quantitative, time-independent parameters of asymmetries in conserved quantum numbers [99, 104]. This framework is particularly useful in analyzing the baryon asymmetry of the Universe, which is marked by the dominance of baryonic matter and the effective absence of antimatter. In the absence of baryon number-violating processes, baryon asymmetry remains conserved within a comoving volume, ensuring that

$$(n_b-n_{\bar{b}})a^3=\text{constant}, \tag{2.77}$$

where n_b and $n_{\bar{b}}$ denote the number densities of baryons and antibaryons, respectively. Using this relation, along with Eq. (2.74), we can immediately see that the ratio

$$B_s\equiv\frac{n_B}{s}, \tag{2.78}$$

where $n_B\equiv n_b-n_{\bar{b}}$, represents a time-independent measure of baryon asymmetry, assuming that the Universe's expansion is isotropic. This assumption holds true with a high degree of precision throughout most of the Universe's history. After photon decoupling, the number of non-interacting photons in a comoving volume remains constant, with the temperature of the photon background T_γ scaling as $T_\gamma\propto a^{-1}(t)$ and the photon number density $n_\gamma\sim a^{-3}(t)$. Consequently, following this period, and provided that no further baryon number-violating processes occur, the ratio n_B/n_γ remains constant.

At higher temperatures, the annihilation of massive particles begins once the temperature drops below their respective masses. These annihilations heat the primordial plasma, leading to an increase in photon number density. Therefore, it is more practical to introduce the quantity B, which remains effectively constant under thermal equilibrium conditions throughout the expansion. In the Standard Model of particle physics, assuming no new long-lived particles, there is no significant transfer of entropy to the photons after the annihilation of e^+e^- pairs, resulting in the constancy of $a^3 n_\gamma$. Therefore, at lower temperatures, particularly below $T \lesssim 1$ MeV, the baryon-to-photon ratio is used

$$\eta \equiv \frac{n_B}{n_\gamma}, \tag{2.79}$$

which also remains constant in this temperature regime and can be related to the quantity B as follows:

$$\eta = \frac{s}{n_\gamma} B_s = \frac{\left(\frac{2\pi^2}{45}\mathcal{S}_{*,0}\right)}{\left(\frac{2\zeta(3)}{\pi^2}\right)} B_s \approx \frac{B_s}{0.14}. \tag{2.80}$$

The baryon-to-photon ratio, η, is approximately ten times the value of B, making the two quantities nearly equivalent. However, at higher temperatures, the baryon-to-photon ratio may deviate by one to two orders of magnitude due to the contributions of heavier particles to the entropy density, which dilutes the ratio by a similar factor. Other sources of dilution may include first- and second-order phase transitions in the early Universe, as well as the out-of-equilibrium decay of unstable particles. These processes can significantly reduce the primordial baryon asymmetry represented by n_B/s.

Current evidence indicates that the present-day baryon asymmetry is approximately [16, 30, 31, 105, 106, 107, 108]

$$\frac{n_B}{s} \sim 9.2 \times 10^{-11}. \tag{2.81}$$

This small value has profound implications for the history of the Universe, particularly by supporting the assumption used in calculating the total entropy density. It also implies that the number density of non-relativistic species, such as protons and neutrons, remains low in the cosmic medium at low temperatures, when these particles become non-relativistic. In the next section this problem will be explored more thoroughly.

Chapter 3

Baryogenesis

From a phenomenological standpoint, the observed baryonic asymmetry represents a major unresolved issue in our understanding of the early Universe. According to the Standard Model (SM) of particle physics, our most robust theoretical framework, the Big Bang should have produced equal quantities of particles and antiparticles. This symmetry would have resulted in their mutual annihilation, leaving behind a Universe composed solely of photons.

In this section, we will introduce the foundational concepts required to address this long-standing problem, and provide the essential frameworks that will underpin the discussions in the subsequent sections.

3.1 Sakharov conditions

In the context of baryogenesis, it is well established that, without imposing certain ad hoc conditions, there is no straightforward solution to the perplexing question of the apparent asymmetry between matter and antimatter in the Universe. A more plausible approach is to assume that this asymmetry was dynamically generated in the early Universe. In this case, the process responsible for creating the asymmetry is referred to as baryogenesis. This was the idea of A.D. Sakharov that proposed that the baryon asymmetry might not result from unnatural initial conditions but could instead be explained through microphysical laws [32]. These laws imply that an initially symmetric Universe could dynamically develop the observed asymmetry, creating a theoretical framework for understanding this phenomenon within particle physics and cosmology. Sakharov outlined a “recipe” for generating this asymmetry, which has become fundamental to the study of baryonic asymmetry. The three conditions defined by Sakharov are:

1. Baryon number violation;
2. Violation of C (charge conjugation symmetry) and CP (the composition of parity and C);
3. Departure from the equilibrium.

The major path to take when building such type of processes is the fulfilment of the *Sakharov conditions*. The first criterion is straightforward: starting from a symmetric Universe, baryon number violation must occur for the Universe to evolve into a state where the baryon-to-photon ratio, η, is non-zero. This violation generates a net baryon number, $\Delta B > 0$, where a simple example of such a process can be represented as $X \to Y + b$, leading to $\Delta B = 1$.

The second Sakharov condition is essential because if charge conjugation (C) and charge-parity (CP) symmetries were preserved, there would be no preference for matter over antimatter. In such a case, baryon number-violating interactions would produce baryons and antibaryons at equal rates, maintaining a net baryon number of zero. In other words, the thermal average of the baryon number operator B, which is odd under both C and CP transformations, remains zero unless these symmetries are violated. To illustrate this, we can compute the thermal equilibrium average of B as follows [109]

$$\langle B\rangle_T = \mathrm{Tr}\left(e^{-\beta H}B\right) = \mathrm{Tr}\left[(CPT)(CPT)^{-1}e^{-\beta H}B\right] = \mathrm{Tr}\left(e^{-\beta H}(CPT)(CPT)^{-1}\right) = -\mathrm{Tr}\left(e^{-\beta H}B\right), \tag{3.1}$$

showing that in equilibrium, $\langle B\rangle_T = 0$, which implies no generation of a net baryon number.

The departure from thermal equilibrium is particularly crucial for the following work. This departure can be driven directly or indirectly by the expansion of the Universe, linking macroscopic cosmological dynamics with the microphysical processes that explain the observed asymmetry between matter and antimatter. As a result, the observed baryon number emerges from the interplay between the laws governing both macroscopic and microscopic phenomena. In thermal equilibrium, the process $X \to Y + b$ is balanced by its inverse process $Y + b \to X$, resulting in no net change in the baryon number. Departure from equilibrium disrupts this balance, allowing for the generation of a non-zero baryon number.

3.2 Baryogenesis mechanisms: Electroweak theory, Grand Unification Theories and Gravity

When talking about baryogenesis mechanisms, there exists a plethora of mechanisms to choose. Most baryogenesis mechanisms depend on physics beyond the Standard Model (for more details, see [110, 111, 112, 113, 114]), highlighting how the baryon asymmetry can serve as a gateway to new physics. The necessity for physics beyond the SM arises not only as a potential solution to the asymmetry problem, where Grand Unified Theories (GUTs) were initially proposed due to their natural inclusion of baryon number violation, but also due to the SM's insufficient CP violation and the limitations of Electroweak Baryogenesis (EWB), a process relying solely on SM interactions [80, 81, 82, 115, 116]. Gravity can also make a crucial contribution to the asymmetry problem, with Gravitational Baryogenesis (GB) [72] being the most well-built mechanism.

In this thesis, these three mechanisms will be explored and their framework will be presented and extended by using modified theories of gravity. This work will be divided into two paths. **Path A** will consist on using a Scalar-Tensor theory in the context of EWB and GUTB. **Path B** will consist in using $f(R,\mathcal{T}^2)$ in the context of GB. The idea behind this stratification is to explore more deeply the role of gravity in the context of baryogenesis where in **Path A** gravity plays a secondary role and on **Path B** is a first-order component.

3.3 Electroweak Baryogenesis

Electroweak baryogenesis is a widely studied and theoretical framework that aims to explain the baryon asymmetry observed in the Universe. As the name suggests, this mechanism postulates that the imbalance between baryons and antibaryons emerged during the electroweak phase transition in the early Universe. In the Standard Model, it was initially believed that two of the Sakharov conditions necessary for baryogenesis were not fulfilled, leading to the conclusion that the SM could not facilitate baryon number violation. This stems from the fact that, at the classical level, baryon number is conserved, as expressed by the conservation laws $\partial_a j_B^a = \partial_a j_L^a = 0$, where $j_B^a = \bar{q}\gamma^a q$ and $j_L^a = \bar{l}\gamma^a l$ represent the baryonic and leptonic vector currents, respectively. These conservation laws imply that the baryonic and leptonic charges, defined as $B = \int d^3x j_B^0$ and $L = \int d^3x j_L^0$, are time-independent. Consequently, baryon number violation does not occur within the SM framework at this classical level. However, when quantum corrections are taken into account, this conservation no longer holds. In regions where quantum fluctuations around the local value of the gauge field, $W_{\bar{\mu}}$, are small, the baryon number change, ΔB, remains zero. Yet, large field configurations can lead to baryon number violation. In 1976, 't Hooft demonstrated that certain special field configurations, known as instantons, allow for tunneling between states with different baryon numbers. Specifically, an instanton can transition from a state $|\varphi, B\rangle$ to a state $|\varphi, B+3\rangle$ with a probability per unit volume proportional to $\langle\varphi, B+3|\varphi, B\rangle \propto e^{-4\pi/\alpha_W} \sim 10^{-164}$, where $\alpha_W = g_W^2/4\pi$ is the weak coupling constant. This result, which applies at zero temperature, explains why baryon-number violation has not been observed experimentally.

However, at finite temperatures, the situation changes. In this case, field configurations known as sphalerons, which are saddle-point solutions of the classical field equations, can transition over the barrier separating vacua. These sphalerons sit atop the energy barrier and are thus "ready to fall,"as their name, derived from Greek, suggests. The rate of such processes is determined by the fluctuations around the sphaleron solution. Arnold and MacLerran calculated the rate per unit volume and unit time as

$$\frac{\Gamma_{\text{sph}}}{V} = a(E_{\text{sph}})^3 m_W(T) \exp\left(-\frac{E_{\text{sph}}}{T}\right), \tag{3.2}$$

where $m_W(T) = g_W v/2$ is the temperature-dependent mass of the W boson, a is a constant, and E_{sph} is the sphaleron energy, given by

$$E_{\text{sph}} = \frac{2m_W(T)}{\alpha_W} B\left(\frac{m_H}{m_W(T)}\right), \tag{3.3}$$

where m_H is the mass of the Higgs boson, and the function B takes values between 1.56 and 2.72. As a result, E_{sph} is on the order of 10 TeV, and thus the sphaleron rate, Γ_{sph}, is typically small at temperatures just below the electroweak phase transition, $T \sim 100$ GeV.

Above the electroweak phase transition, before symmetry breaking occurs and the Higgs boson is in its symmetric vacuum, the W boson mass vanishes. Dimensional analysis suggests that, in this regime, the sphaleron rate scales as $\Gamma_{\text{sph}}/V \sim \kappa\alpha_W^4 T^4$, and lattice some computations have refined this to $\Gamma_{\text{sph}} = (25.4 \pm 2.0)\alpha_W^5 T^4$. By considering the thermal volume $V = T^{-3}$, the sphaleron rate is found to be $\Gamma_{\text{sph}} \simeq 10^{-6} T$. Comparing this rate with the expansion rate of the Universe gives a temperature threshold of $T_* \simeq 10^6 g_*^{-1/2}(T) m_{\text{Pl}} \simeq 10^{12}$ GeV. Consequently, sphaleron processes come into equilibrium when the temperature drops below this value. If no net $B-L$ asymmetry exists at that time, the sphaleron processes will wash out any existing baryon or lepton number.

3.3.1 The Electroweak Baryogenesis Mechanism

For Electroweak Baryogenesis (EWB) to occur, the initial conditions assumed are a hot, radiation-dominated early Universe with zero net baryon charge, where the full $SU(2)_L \times U(1)_Y$ electroweak symmetry is preserved [81, 117, 118, 119, 120]. As the temperature of the Universe drops below the electroweak scale, the electroweak symmetry spontaneously breaks because of the Higgs field settling into a vacuum state. During this phase transition, the baryogenesis process occurs.

Theoretically, this phase transition proceeds as bubbles of the broken phase nucleate within the plasma, which is still in the symmetric phase. These bubbles expand, collide, and eventually coalesce, leaving behind only the broken phase [81, 121]. The production of baryons as the bubble wall sweeps through space can be categorized into two distinct mechanisms [109]:

1. *Nonlocal baryogenesis*: Particles interact with the bubble wall in a manner that violates CP symmetry, generating an asymmetry in a quantum number other than the baryon number in regions of the unbroken phase, away from the wall. Baryon-number violating processes then convert this pre-existing asymmetry into a baryon number asymmetry, leading to the generation of baryons (see [122, 123] for more details).

2. *Local baryogenesis*: Baryons are produced when baryon number and CP-violating processes take place together near the bubble walls.

In general, both mechanisms will contribute to the baryon asymmetry, and the total asymmetry will be the sum of the contributions from both processes. However, there are conditions that determine which mechanism dominates. If the speed of the bubble wall exceeds the speed of sound in the plasma, local baryogenesis dominates. Otherwise, nonlocal baryogenesis is typically more efficient [109].

3.3.2 The conditions for a successful EWB: the Sphaleron Bound

In order for any model of Electroweak Baryogenesis that proceeds via the bubble wall scenario to be considered successful, it must satisfy two essential requirements that have a deep connection with the asymmetry production and the departure from equilibrium. First, sphaleron processes must be effective in the symmetric phase to ensure that sphaleron transitions are in equilibrium and that baryon number violation is fully efficient outside the bubble. Second, it must be guaranteed that sphaleron processes become ineffective after the completion of the phase transition so that the previously generated asymmetry does not get diluted.

The fulfillment of the first requirement can be examined by comparing the rate of baryon number non-conserving processes in the symmetric phase to the expansion rate. The thermal rate per unit volume of sphaleron events, as given by [109], is

$$\Gamma_{\rm sph}^{\rm sym}(T) = \kappa(\alpha_W T)^4. \tag{3.4}$$

This can be expressed as

$$V_B^{\rm sym} = \frac{\mathcal{M}}{T^3}\Gamma_{\rm sph}^{\rm sym} = \mathcal{M}\kappa\alpha_W^4 T, \tag{3.5}$$

where $\mathcal{M} = \frac{13}{2n_f}$. The prefactor κ was calculated in [124] and was found to have an additional dependence on α_W, such that $\kappa \approx 25\alpha_W$. Using this result, the equilibrium condition for sphaleron transitions in the symmetric phase ($V_B^{\rm sym}(T) > H(T)$) is satisfied if

$$T < 7.53\mathcal{M}\alpha_W^5 \frac{M_{Pl}}{\sqrt{g_*}}, \tag{3.6}$$

where $T_{\rm sph}$ is defined as

$$T_{\rm sph} \equiv 7.53\mathcal{M}\alpha_W^5 \frac{M_{Pl}}{\sqrt{g_*}}. \tag{3.7}$$

For the Standard Model, with $g_* = g_{SM} = 106.75$, this yields $T_{\rm sph} \approx 7.5\times 10^{12}$ GeV. Therefore, the temperature at which sphaleron processes reach equilibrium is very high and is not a significant concern.

The second requirement is somewhat different and is a criterion that must be met for the bubble-wall scenario to be successful. To have such a scenario, one must ensure that the electroweak phase transition is a strong first-order phase transition [80, 81, 82]. To determine the bound for this criterion, one begins with the master equation which can be expressed as

$$\frac{dN_B}{dt} = -n_f^2 \frac{\Gamma_{\text{sph}}}{T} \frac{\partial F}{\partial(N_B + N_L)} = -n_f^2 \frac{\Gamma_{\text{sph}}}{T} (\mu_B + \mu_L), \tag{3.8}$$

where μ_B and μ_L denote the chemical potentials for baryon number B and lepton number L, respectively. Assuming $B - L = 0$, $\mu_B + \mu_L$ can be computed (see [125]) as

$$\mu_B + \mu_L = \frac{13}{2} \frac{N_B}{n_f} T^{-2}. \tag{3.9}$$

Substituting this result into the master equation and integrating formally yields

$$\frac{N_{B_f}}{N_{B_C}} = \exp\left[-\frac{13}{2} n_f \int_{t_{Cr}}^{t_f} \frac{\Gamma_{\text{sph}}(T(t'))}{T(t')^3} dt'\right], \tag{3.10}$$

where t_{Cr} represents the time at which bubble nucleation begins and t_f denotes the time at which sphaleron processes cease to be effective. Here, N_{B_f}/N_{B_C} represents the dilution of the baryon asymmetry, with N_{B_f} being the final asymmetry to be preserved until the present day.

The thermal rate per unit time and volume for fluctuations between neighboring minima, given by [109], is

$$\Gamma_{\text{sph}}^{\text{bro}}(T) = \mu \left(\frac{M_W}{\alpha_W T}\right)^3 M_W^4 \exp\left(-\frac{E_{\text{sph}}(T)}{T}\right). \tag{3.11}$$

This can be rewritten in terms of the sphaleron energy as

$$\begin{aligned} \Gamma_{\text{sph}} &= 2\pi^4 \mu T^4 \left(\frac{\alpha_W}{4\pi}\right)^4 \left(\frac{E_{\text{sph}}(T)}{BT}\right)^7 \exp\left[-\frac{E_{\text{sph}}(T)}{T}\right] \\ &\approx 2.8 \times 10^5 \kappa T^4 \left(\frac{\alpha_W}{4\pi}\right)^4 \left(\frac{E_{\text{sph}}(T)}{BT}\right)^7 \exp\left[-\frac{E_{\text{sph}}(T)}{T}\right], \end{aligned} \tag{3.12}$$

where the approximation in the final step is from reference [126], and the prefactor κ was found to be in the range $10^{-4} \lesssim \kappa \lesssim 0.1$ [127]. For simplicity, let us define the rate for baryon non-conserving processes as

$$V_B(T) \equiv \mathcal{M} \frac{\Gamma_{\text{sph}}}{T^3}. \tag{3.13}$$

Substituting this definition into the integral in Eq. (3.10) and making some assumptions, one obtains a simplified expression. Specifically, since the dominant contribution to the integral comes from temperatures very close to T_{Cr}, and transitions at lower temperatures are highly suppressed by the exponential factor, one can approximate the integral by evaluating the integrand at $T = T_{Cr}$:

$$\ln\left(\frac{N_{B_f}}{N_{B_C}}\right) = -V_B(T_{Cr})(t_f - t_{Cr}). \tag{3.14}$$

Defining the dilution as $\mathcal{S} \equiv \frac{N_{B_f}}{N_{B_C}} = \frac{n_{B_f}/s_0}{n_{B_C}/s_C}$, where s_0 is the entropy at the present time, $s_C \equiv s(t_{Cr})$ is the entropy at the time of the phase transition, and $n_{B_f} = n_B(t_f)$ is the baryon-to-entropy density ratio observed today, the maximum allowable dilution that preserves the observed baryon density is given by $\mathcal{S}_{\max} \sim 7 \times 10^{-11} \frac{s_C}{n_{B_C}}$. Consequently, the baryon asymmetry produced at the electroweak phase transition, $\frac{n_B}{s_C}$, remains an open question. However, generating a large asymmetry is generically difficult and is very unlikely to exceed 10^6. Hence, one can reasonably set the bound $N_{B_C} \lesssim 10^6$. To prevent baryon asymmetry from being washout, the requirement $S \gtrsim 10^{-5}$ must be met.

In standard cosmology, the time-temperature relation for a radiation-dominated Universe is given by $t = 0.301 g_*^{-1} M_{Pl} T^{-2}$. Therefore,

$$t_f - t_{Cr} = 0.301 M_{Pl} \left[g_*(T_{Cr})^{-1} T_{Cr}^{-2} - g_*(T_f)^{-1} T_f^{-2} \right] \approx 0.301 M_{Pl} \frac{T_{Cr}^{-2}}{g_*(T_{Cr})}, \tag{3.15}$$

where $T_f \approx 0$ implies integrating until $t_f = \infty$. Using the relation between $\phi(T_{Cr})$ and $E_{\rm sph}(T_{Cr})$ [126],

$$\frac{\phi(T_{Cr})}{T_{Cr}} = \frac{g}{4\pi B} \frac{E_{\rm sph}(T_{Cr})}{T_{Cr}}, \tag{3.16}$$

and assuming $t_{Cr} - t_f = 0.301 M_{Pl} T_{Cr}^{-2} / g_*(T_{Cr})$, the sphaleron bound can be written as

$$\sqrt{\frac{4\pi}{\alpha_W}} \frac{\phi_{Cr}}{T_{Cr}} B - 7 \ln \left(\sqrt{\frac{4\pi}{\alpha_W}} \frac{\phi_{Cr}}{T_{Cr}} B \right) \gtrsim \ln \left[\frac{2.8 \times 10^5 \kappa \mathcal{M}}{5 \ln 10 \times B^7} \left(\frac{\alpha_W}{4\pi} \right)^4 \right] + \ln \left(\frac{T_{Cr}}{2 H_{Cr}} \right), \tag{3.17}$$

where $\phi_{Cr} \equiv \phi(T_{Cr})$ and $H_{Cr} \equiv H(T_{Cr})$ is the standard cosmology expansion rate for a radiation-dominated Universe at the time of the phase transition. The parameter B as a function of the Higgs mass m_H is approximated by [126] as

$$B \left(\frac{m_H}{m_W} \right) \simeq 1.58 + 0.32 \left(\frac{m_H}{m_W} \right) - 0.05 \left(\frac{m_H}{m_W} \right)^2, \tag{3.18}$$

valid for 25 GeV $\leq m_H \leq$ 250 GeV. This parameter ranges from $B(0) = 1.52$ to $B(\infty) = 2.70$ [128, 129, 130, 131]. For $T_{Cr} = 10^2$ GeV, $n_f = 3$, $\alpha_W = 0.0336$, $\kappa = 0.1$, and $B = 1.9$, the sphaleron bound in Eq. (3.17) can be numerically solved to give

$$\frac{\phi_{Cr}}{T_{Cr}} \gtrsim 1.22\,. \tag{3.19}$$

As previously mentioned, this condition is essential for the success of Electroweak Baryogenesis (EWB). Failure to meet this requirement compromises the viability of the mechanism. Unfortunately, current observations suggest that this is the case for EWB. Recent measurements of the Higgs mass indicate that the Electroweak Phase Transition is not a strong first-order transition, but rather a smooth crossover [132, 133, 134, 135, 136]. This limitation has long been a significant challenge for the EWB mechanism. A common solution has been to introduce additional and more complex sectors to the SM. However, in [137], an alternative approach was proposed, focusing instead on modifying the cosmological description. Specifically, it was suggested that the Universe could be dominated by the kinetic energy of a scalar field, which scales as $a^{1/6}$. In the same line of reasoning, this thesis will explore the use of modified gravity with the goal of relaxing the constraint in question as the sphaleron bound has a relation with the expansion rate of the Universe.

3.4 GUT Baryogenesis

The primary objective of Grand Unified Theories (GUTs) is to integrate the strong, weak, and electromagnetic forces, as well as quarks and leptons, within the framework of gauge field theory based on a non-Abelian symmetry group [138, 139, 140, 141]. A key feature of GUTs is the placement of leptons and baryons in the same multiplets, leading to their mixing under gauge transformations. Consequently, baryon and lepton numbers are not independently conserved, enabling interactions that violate baryon number, such as $e^- + d \leftrightarrow \bar{u} + \bar{u}$ or decays of superheavy gauge (or Higgs) bosons, for example $X \to e^- + d + \bar{u} + \bar{u}$. To elucidate the mechanisms of baryon number violation, consider a scenario where $X, \bar{X}, q, \bar{q}, l$, and $\bar{l}$ represent an arbitrary superheavy gauge boson, its antiparticle, a quark, an antiquark, a lepton, and an antilepton, respectively. Given that the decays of superheavy bosons are central to baryogenesis, the following discussion will focus on this topic. Superheavy bosons, such as X, have decay modes of the form $X \to ql$ and $X \to \bar{q}\bar{q}$, while their antiparticles $\bar{X}$ can decay via $\bar{X} \to \bar{q}\bar{l}$ and $\bar{X} \to qq$ (for more details [96, 142]). These decays explicitly violate baryon number, thus satisfying the first of Sakharov's conditions for baryogenesis. More specifically, if we denote the branching ratios of the various decay modes of X and $\bar{X}$ as r, $1-r$, $\bar{r}$, and $1-\bar{r}$, the net baryon number produced by the decay of an X boson is given by $B_X = r/3 - 2(1-r)/3$, and for an $\bar{X}$ boson, it is $B_{\bar{X}} = -\bar{r}/3 + 2(1-\bar{r})/3$. Therefore, the total net baryon number produced by the decay of an X and $\bar{X}$ pair is $\varepsilon = B_X + B_{\bar{X}} = r - \bar{r}$.

To further explore this, consider the decay channel $X \to \bar{q}\bar{l}(1)$, where the parity (P) of state (1) is denoted as $(\uparrow)$ or $(\downarrow)$. The following transformation properties can be written

$$\begin{aligned} &\text{Under CPT:} && \Gamma(X \to 1\uparrow) = \Gamma(\bar{1}\downarrow \to \bar{X}), \\ &\text{Under CP:} && \Gamma(X \to 1\uparrow) = \Gamma(\bar{X} \to \bar{1}\downarrow), \\ &\text{Under C:} && \Gamma(X \to 1\uparrow) = \Gamma(\bar{X} \to \bar{1}\uparrow), \end{aligned} \tag{3.20}$$

where Γ represents the decay width of X to a ql state. From this we can conclude [96]

$$\varepsilon = r - \bar{r} = \Gamma(X \to 1\uparrow) + \Gamma(X \to 1\downarrow) - \Gamma(\bar{X} \to \bar{1}\uparrow) - \Gamma(\bar{1}\downarrow). \tag{3.21}$$

This result holds regardless of the specific choice for state (1). However, it is evident that if charge conjugation (C) or combined charge-parity (CP) symmetry is preserved, then $\varepsilon = 0$. Thus, two additional conditions must be met for baryogenesis: violation of C and CP, as well as departure from thermal equilibrium. While CP violation in GUTs can be a complex topic, this discussion will focus on the necessary departure from equilibrium and the mechanism of Non-Inflationary GUT-Baryogenesis.

3.4.1 Departure from equilibrium and Inflation

The third Sakharov criterion is satisfied when the Universe's expansion rate surpasses the rate of particle interactions. Essentially, the critical factor is the comparison between cosmic expansion and microphysical processes. In the early Universe, when the bosons responsible for baryon non-conserving processes are still relativistic, they remain in thermal equilibrium, with their number density given by $n_X = n_{\bar{X}} = (g_X/g_\gamma)n_\gamma = (\zeta(3)/\pi^2)g_X T^3$. Here, symmetric initial conditions imply equal numbers of X and $\bar{X}$ bosons. As the temperature drops, these numbers stay in equilibrium only if creation and annihilation processes, like decays and inversions, proceed faster than the cosmic expansion rate, i.e., $\Gamma \gtrsim H$. If particle interactions slow down relative to expansion ($\Gamma \lesssim H$), the bosons decouple, and their numbers "freeze out,"remaining comparable to the photon count. For sufficiently massive bosons, annihilation and decay become inefficient when $T < m_X$, causing the number of X and $\bar{X}$ bosons to deviate from equilibrium. This leads to an overabundance, with $n_X \simeq n_{\bar{X}} \simeq n_\gamma \gg n_X^{\text{eq}} = n_{\bar{X}}^{\text{eq}} = (m_X T)^{3/2}\exp(-m/T)$. This excess creates the out-of-equilibrium condition necessary for generating baryon asymmetry, as the heavy X particles undergo baryon- (B) and charge-parity- (CP) violating decays. Given these decays proceed via renormalizable operators, very heavy particles are required, with masses $m_X \gtrsim 10^{15} - 10^{16}$ GeV for gauge bosons, and $m_X \gtrsim 10^{10} - 10^{16}$ GeV for scalar bosons [96, 109]. Annihilation becomes limited by the particle number, $\Gamma_{\rm ann} \propto n_X$, while decay processes maintain equilibrium. For simplicity, annihilation is neglected in this analysis.

In scenarios where inflation is not included, as inflation carries the risk to "washout" the asymmetry produced, it is generally assumed that the early Universe was filled with a hot, dense mixture of all fundamental particles in thermal equilibrium, including the supermassive bosons responsible for baryon-nonconserving processes. This assumption is a critical aspect of the model. Several processes involving superheavy bosons can impact the final value of baryon asymmetry. To leading order in α_S, these processes include the decays and inverse decays of superheavy bosons (order α_S), baryon-nonconserving fermion collisions (BNC-scattering processes), and Compton-type or annihilation-like reactions (both of order α_S^2). Typically, second-order processes are insignificant, and higher-order processes are generally negligible [143]. However, among the second-order processes, BNC-scattering is the most likely to be relevant in certain situations. Any process besides decay will only serve to dampen the generation of asymmetry produced by the decays themselves. The effectiveness of these damping processes in counteracting the decays depends on their rates relative to the expansion rate of the Universe. If we consider only decay, inverse decay, and BNC-scattering processes, the departure from thermal equilibrium can be quantified by calculating the rates of each process. Formal derivations of these rates are provided in [96, 143]. They are expressed as follows

$$\Gamma_D \simeq \alpha_X \frac{m_X^2}{\sqrt{T^2+m_X^2}} \simeq \begin{cases} \alpha_X m_X^2/T & \text{if } T \gtrsim m_X, \\ \alpha_X m_X & \text{if } T \lesssim m_X, \end{cases} \tag{3.22}$$

$$\Gamma_{ID} \simeq \Gamma_D X^{\rm eq} \simeq 2\Gamma_D \begin{cases} 1 & \text{if } T \gtrsim m_X, \\ \sqrt{\pi/8}(m_X/T)^{3/2}\exp(-m_X/T) & \text{if } T \lesssim m_X, \end{cases} \tag{3.23}$$

$$\Gamma_S \simeq A\alpha_X^2 \frac{T^5}{(T^2+m_X^2)^2} \simeq A\alpha_X^2 \begin{cases} m_X T & \text{if } T \gtrsim m_X, \\ T^5/m_S^4 & \text{if } T \lesssim m_X, \end{cases} \tag{3.24}$$

where $X^{\rm eq}$ represents the equilibrium number of X bosons, Γ_{ID} corresponds to the inverse decay rate, and Γ_S refers to the BNC-scattering rate. The constant A is a numerical factor, on the order of 10^3, accounting for the number of available scattering channels, among other factors.

For baryogenesis, the most critical rate is the decay rate Γ_D, as decays primarily regulate the number of X and $\bar{X}$ bosons. Decay processes dominate the reduction of superheavy boson numbers, as annihilation processes are of higher order (α^2). Given that these bosons mediate baryon nonconservation, their decay plays a central role in the process.

To assess the effectiveness of these decay and inverse decay processes, we define the quantity

$$K \equiv \left(\frac{\Gamma_D}{2H}\right)_{T=m_X} = 3.68\times 10^{18}\frac{\alpha_X}{\sqrt{g_{*S}}}\frac{\rm GeV}{m_X}, \tag{3.25}$$

where K measures the effectiveness of decays (Γ_D/H), inverse decays (Γ_{ID}), and, inversely proportional to α, the effectiveness of BNC-scattering processes ($\Gamma_S/H\alpha$) at the crucial moment when the bosons X become non-relativistic ($T = m_X$). At this point, the bosons must undergo a rapid reduction in number to remain in equilibrium.

With the previous framework defined, we have all the tools to work with GUTB in the context of modified gravity aiming to see how MG can help GUTB.

3.5 Gravitational Baryogenesis

Gravitational baryogenesis is a proposed mechanism for generating baryon asymmetry while preserving thermal equilibrium. It involves an interaction term given by [72]

$$\mathcal{L}_{int} = \frac{1}{M_*^2}\partial_\mu(R)J_B^\mu\,, \tag{3.26}$$

where $\partial_\mu(R)$ represents the derivative of the Ricci scalar R, and J_B^μ denotes the baryon number current. In an expanding universe, this term can lead to violations of CP and CPT symmetries by directly coupling the Ricci scalar with the baryon number current. This interaction can also be extended to lepton currents or any current associated with a net $B-L$ charge in equilibrium. The parameter M_*^2 represents the cutoff scale of the effective theory and it is hypothesized that this interaction originates from a higher-dimensional operator in supergravity theories [144, 145]. Moreover such operators may appear in a low-energy effective field theory of quantum gravity, particularly if the fundamental scale M_* is close to the reduced Planck scale $M_{Pl} \approx 2.4\times 10^{18}$ GeV [72].

A distinguishing feature of this mechanism is that CP violation originates from gravitational interactions. As the universe expands, microscopic CP violation is magnified due to changes in baryon energy, which leads to dynamic CPT violation that affects the energy distributions of particles and antiparticles. Consequently, a CP-conserving but baryon number-violating interaction in equilibrium can generate the baryon asymmetry, which is enhanced by the interaction term and becomes fixed once the baryon number-violating interactions decouple. To quantify this, in a flat Friedmann-Lemaître-Robertson-Walker universe with spatially constant R, the interaction term induces differential energy contributions for baryons and anti-baryons, modifying their thermal equilibrium distributions as follows [72, 146]

$$\frac{1}{M_*^2}(\partial_\mu R)J_B^\mu = \frac{1}{M_*^2}\dot{R}(n_B - n_{\bar{B}})\,, \tag{3.27}$$

where $J_B^0 = n_B - n_{\bar{B}}$, with n_B and $n_{\bar{B}}$ representing the number densities of the baryon and antibaryon, respectively. This results in a shift in baryon energy of approximately $\frac{2\dot{R}}{M_*^2}$ relative to anti-baryons, leading to CPT symmetry violation. Consequently, the chemical potential for baryons is given by $\mu_B = -\mu_{\bar{B}} = -\frac{\dot{R}}{M_*^2}$. In an expanding Universe, considering the relativistic regime ($T \gg m$) and $T \gg \mu_B$, using Eq.(2.56) for fermions and Eq.(2.68) the asymmetry produced by the interaction given in Eq.(3.26) at the temperature where the baryon number violation processes decouple, T_D, is given by [72]

$$\frac{n_b}{s} \simeq -\frac{15 g_b}{4\pi^2 g_*}\frac{\dot{R}}{M_*^2 T}\bigg|_{T_D}\,, \tag{3.28}$$

where $\dot{R}$ is determined based on the cosmological model used. In essence, the coupling term in (3.26) modifies the thermal equilibrium distribution and the chemical potential, driving the universe toward a nonzero equilibrium B-asymmetry (or L-asymmetry) through B-violating (or L-violating) interactions. This mechanism is closely related to spontaneous baryogenesis [147, 148], where, in the case of gravitational baryogenesis, the Ricci scalar from a gravitational background takes on the role usually filled by an axion in spontaneous baryogenesis. In spontaneous baryogenesis, the symmetry that guarantees baryon number conservation in the unbroken phase is spontaneously broken. Upon symmetry breaking,

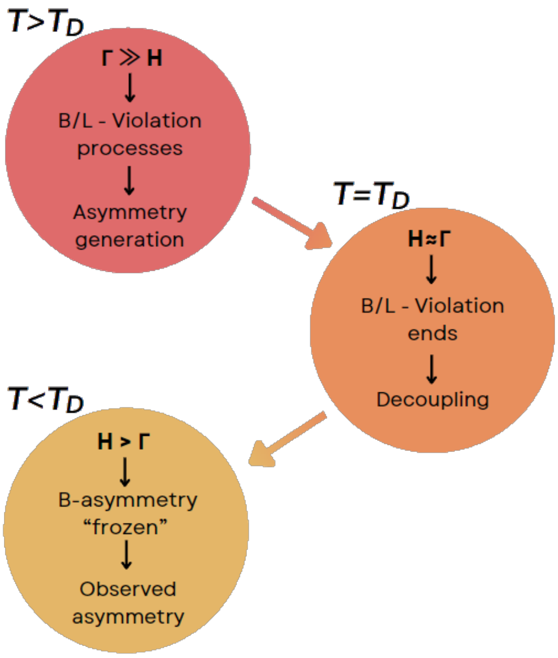

Figure 3.1: Schematic representation of the generation of baryon asymmetry in the regime of thermal equilibrium. Image taken from arXiv:2409.04623 [gr-qc].

the Lagrangian density acquires an additional term [147, 148, 149]

$$\mathcal{L} = \frac{(\partial_\mu \phi)}{f} J^\mu_B \,, \tag{3.29}$$

where ϕ is typically a pseudo-Nambu-Goldstone boson associated with an approximate symmetry related to the baryon number, and f is a parameter linked to the scale of symmetry breaking.

Both of these mechanisms can occur if the baryon number-violating processes occur in thermal equilibrium. In an expanding Universe, the generation of baryon asymmetry within thermal equilibrium follows a specific sequence. During periods when the expansion rate H significantly surpasses the interaction rate Γ,i.e., when $\Gamma \gg H$, corresponding to temperatures $T > T_D$, baryon asymmetry is produced by processes that violate either baryon number (B) or lepton number (L), all while maintaining thermal equilibrium. As the temperature decreases to $T = T_D$, where $H \approx \Gamma$, these processes decouple. Once $H < \Gamma$, or $T < T_D$, the baryon asymmetry becomes effectively frozen. This process is schematically illustrated in Fig. 3.1. This feature is particularly noteworthy as it challenges the Sakharov conditions. In fact, these conditions are not strictly necessary [147, 150, 151, 152, 153] but are a fundamental framework of baryogenesis. This phenomenon has been widely studied in the context of spontaneous baryogenesis [147, 148], which requires only the violation of baryon number (B) while remaining in thermal equilibrium. Under such conditions, spontaneous baryogenesis is typically more efficient.

For this thesis, gravitational baryogenesis will be explored in the context of modified theories of gravity as from a phenomenological perspective, modifying gravitational baryogenesis offers solutions to several challenges present in its original formulation. One prominent issue is the difficulty in generating a non-zero asymmetry during the radiation-dominated era, where the equation of state is characterized by $w = 1/3$. However, this problem can be mitigated by considering deviations where $w \approx 1/3$ [72]. Additionally, as already mentioned in the Introduction, modified gravitational baryogenesis can address scenarios where the generated asymmetry is either too small or excessive. This approach may also help to resolve intrinsic issues, such as the instabilities [153, 154, 155]. The modified theory of gravity chosen was $f(R,\mathcal{T}^2)$ as it is a non-minimally geometry-matter coupled (NMGM) theory that brings a more impactful role of matter in to the cosmological description as we will see later on. Another rational behind the choice of this theory is the fact that in theories in which matter and geometry are non-minimally coupled, one interesting feature is the non-conservation of the matter energy-momentum tensor $\nabla^{\mu}T_{\mu\nu} \neq 0$ [156, 157, 158, 159]. This feature can be seen from a thermodynamic perspective as describing irreversible processes of matter creation [160, 161] and recently this phenomenology was explored in [162].

The concept of gravitationally-induced particle production offers a compelling reason to investigate the direct coupling of matter-related quantities with the baryonic current. However, it is important to clarify that in this context, gravitational particle production is not used directly to generate baryonic asymmetry. More interestingly, this mechanism, which emerges from the non-conservation of the energy-momentum tensor in theories involving geometry-matter couplings, can be combined with gravitational baryogenesis to achieve the desired baryonic asymmetry. This combination requires careful attention to various factors, such as ensuring entropy conservation after the baryogenesis epoch and devising a mechanism to produce more particles than antiparticles through a B-violating process, which may or may not involve gravitational particle creation. In gravitational baryogenesis, despite the "gravitational"label, gravity does not directly induce B or B-L violation. Instead, gravity affects the net baryon current via the cosmological background, while the resulting baryon asymmetry depends on an existing B-violating process. The interaction term from Eq. (3.26) amplifies the baryon asymmetry to its observed value, which becomes fixed once the B-violating processes decouple. Consequently, a mechanism that utilizes gravitational particle production to generate baryonic asymmetry, coupled with a B-violating process potentially linked to gravitational effects, and subsequently amplifies this asymmetry through gravitational baryogenesis, can be considered primarily gravitational in nature. This holds true even when additional mechanisms contribute to the asymmetry.

A similar idea was explored in [163], where GR was employed to describe the gravitational dynamics, resulting in a different rationale for gravitational particle production than the approach discussed here. More recently, in [164], a related mechanism was proposed that integrates Cosmological Gravitational Particle Production (CGPP) [165], which combines cosmic inflation, quantum field theory, general relativity, and particle physics, with baryogenesis arising from Grand Unified Theories.

Chapter 4

Modified theories of gravity

In this chapter, we introduce alternative theories to General Relativity, often referred to in the literature as modified gravity theories. A concise overview will be provided, with a focus on scalar-tensor theories and theories involving non-minimal couplings between geometry and matter, more specifically $f(R,\mathcal{T}^2)$, where $\mathcal{T}^2 \equiv T_{\mu\nu}T^{\mu\nu}$. These approaches offer a range of possibilities for addressing limitations of General Relativity, particularly for the previous problems mentioned. The relation between inflation and scalar-tensor theories will also be briefly mentioned. This chapter is based on [116, 146].

4.1 Scalar-Tensor theories

When extending Einstein's General Relativity while preserving its metric framework, Scalar-Tensor Theories (STT) assume a central role. These theories introduce an additional scalar field to mediate gravitational interactions alongside the metric tensor field. A notable example is the Brans-Dicke theory, introduced in 1961 [60] having the action

$$S_{\rm BD} = \frac{1}{16\pi}\int_{\mathcal{M}} \sqrt{-g}\,\mathrm{d}^4x \left[\phi R - \frac{\omega_{BD}}{\phi} g^{\mu\nu}\partial_\mu\phi\partial_\nu\phi\right] + S_M \ , \tag{4.1}$$

with ω_{BD} being a dimensionless constant, ϕ plays a role analogous to G^{-1} and S_M being the usual action related to the matter sector that does not contain the scalar field ϕ. Later this theory was generalized by Bergmann [166], Wagoner [167], and Nordtvedt [168] to include arbitrary coupling parameters. Currently, the fundamental action for STTs is expressed as

$$S_{\rm STT} = \frac{1}{16\pi}\int_{\mathcal{M}} \sqrt{-g}\,\mathrm{d}^4x \left[\phi\left[R - 2\lambda(\phi)\right] - \frac{\omega(\phi)}{\phi} g^{\mu\nu}\partial_\mu\phi\partial_\nu\phi\right] + S_M \ , \tag{4.2}$$

where $\omega(\phi)$ is a dimensionless function representing the coupling between the scalar field and gravity (referred to as the *coupling parameter*), and $\lambda(\phi)$ is another function of the scalar field that can be interpreted as both a potential for ϕ and a cosmological parameter (for this work we will set $\lambda(\phi) = 0$). In this framework, the scalar field ϕ acts as an effective gravitational constant $G_{\rm eff}$[1]. Due to the presence of a non-zero kinetic term ($g^{\mu\nu}\phi_{,\mu}\phi_{,\nu}$) in the action, ϕ is no longer constant but a dynamical variable with

[1] The relation between the scalar field ϕ and the Newton's gravitational constant, that we are familiar with and it is measured in the Cavendish experiment, is subtle. For both BD gravity and STT, one could define an effective gravitational constant $G_{\rm eff} \equiv G_N/\phi$ where G_N is the gravitational constant normalized to its present value, which in what follows will be set as 1 [169]. However, this definition does not lead to be the coupling as measured by the Cavendish experiment. Instead, the latter is given by: $G_* = (G_N/\phi)(2w\phi + 2/2w\phi + 3)$ [169, 170].

dimensions of squared mass. STTs might be seen as emerging from the low-energy limit of superstring theory, where the Brans-Dicke field could be related to the dilaton [171, 172].

Unlike GR, where gravity is mediated solely by the metric tensor $g_{\mu\nu}$, STT involves both the metric tensor and the scalar field ϕ, therefore, when varying the action one must do it with respect to the metric tensor, $\delta g^{\mu\nu}$, yielding a field equation, and also varying it with respect to the scalar field, $\delta\phi$, providing an additional equation of motion. Varying (4.2) with respect to the inverse metric gives (see [173, 174] for a more step by step derivation)

$$\delta S_{\mathrm{STT}} = \frac{1}{16\pi}\int_{\mathcal{M}} \mathrm{d}^4x\sqrt{-g}\delta g^{\mu\nu}\left[\phi G_{\mu\nu} - (\nabla_\mu\nabla_\nu - g_{\mu\nu}\Box)\phi - H^{(\phi)}_{\mu\nu} - 8\pi T_{\mu\nu}\right], \tag{4.3}$$

that leads to the field equation

$$G_{\mu\nu} = \frac{1}{\phi}(\nabla_\mu\nabla_\nu - g_{\mu\nu}\Box)\phi + \frac{1}{\phi}H^{(\phi)}_{\mu\nu} + 8\pi\frac{T_{\mu\nu}}{\phi}, \tag{4.4}$$

where $\Box \equiv \nabla_\mu\nabla^\mu$ is the D'Alembert operator, $G_{\mu\nu}$ is the Einstein's tensor as defined in Eq.(1.62) and $H^{(\phi)}_{\mu\nu}$ can be seen as the stress-energy tensor of the ϕ-field being defined as

$$H^{(\phi)}_{\mu\nu} \equiv \frac{\omega(\phi)}{\phi}\left(\partial_\mu\phi\partial_\nu\phi - \frac{1}{2}g_{\mu\nu}\partial^\alpha\phi\partial_\alpha\phi\right), \tag{4.5}$$

and $T_{\mu\nu}$ is the usual stress-energy tensor defined in Eq.(1.65). During the calculation of the variation in (4.3) we have taken into account the typical requirement that any variations in any field, as well as variations of their first derivatives, vanish on the integration boundary $\partial\mathcal{M}$. Varying now (4.2) with respect to ϕ gives

$$\delta_\phi S_{\mathrm{STT}} = \frac{1}{16\pi}\int_{\mathcal{M}} \mathrm{d}^4x\sqrt{-g}\delta\phi\left[R + 2\omega\frac{\Box\phi}{\phi} - \frac{\omega - \phi\omega'}{\phi^2}\partial_\alpha\phi\partial^\alpha\phi\right]. \tag{4.6}$$

resulting in the modified classical Klein-Gordon equation

$$\Box\phi = \frac{1}{2\omega(\phi)+3}\left[8\pi T - g^{\mu\nu}\partial_\mu\omega\partial_\nu\phi\right], \tag{4.7}$$

where it was used the trace of Eq.(4.4) and with $T \equiv g^{\mu\nu}T_{\mu\nu}$. It can be seen from the Klein-Gordon equation (4.7) that by allowing $\omega(\phi)$ to tend to ∞, the right side of the equation may vanish. This will be the case when ω dominates over $\omega'(\phi)$. In this case, a solution of the type $\phi = constant$, which corresponds to GR, is then admitted by the wave equation (4.7). Therefore, was usually admitted that GR is recovered in the $\omega \to \infty$ of the scalar tensor theories and the value of ω was related to the degree of departure from GR of a scalar tensor theory. However, it was been pointed out that whenever the energy-momentum trace is vanishing (the case of radiation and vacuum) this may not be the case and GR can be fully recovered for a finite ω [175].

4.1.1 Cosmology in STT

To derive cosmological solutions for scalar tensor theories (STT) [176], we employ the field equations (4.4) in conjunction with Eq. (4.7). As presented before, we assume a Universe governed by the FLRW metric, with matter content modeled as a perfect fluid satisfying the barotropic equation of state

(2.8). With this being said, one obtains

$$\left(\frac{\dot{a}}{a}\right)^2+\frac{\dot{a}}{a}\frac{\dot{\phi}}{\phi}+\frac{k}{a^2}-\frac{\omega(\phi)}{6}\frac{\dot{\phi}^2}{\phi^2}=\frac{8\pi}{3}\frac{\rho}{\phi}, \tag{4.8}$$

$$\frac{\ddot{a}}{a}-\frac{\dot{a}}{a}\frac{\dot{\phi}}{\phi}-\frac{1}{2}\frac{\dot{\omega}(\phi)}{2\omega(\phi)+3}\frac{\dot{\phi}}{\phi}=-\frac{8\pi}{3}\frac{\rho}{\phi}\frac{(3\gamma-2)\,\omega(\phi)+3}{2\omega(\phi)+3}-\frac{\omega(\phi)}{3}\frac{\dot{\phi}}{\phi}, \tag{4.9}$$

$$\ddot{\phi}+\left[3\frac{\dot{a}}{a}+\frac{\dot{\omega}(\phi)}{2\omega(\phi)+3}\right]\dot{\phi}=\frac{8\pi\rho}{2\omega(\phi)+3}(4-3\gamma)\,. \tag{4.10}$$

To fulfill path A, we will adopt the three-epoch model discussed in [177, 178] and used in [116], and we refer the reader to these sources for a comprehensive examination of the model's intricacies. Initially, the model assumes that the Universe is described by an FLRW metric and an energy-momentum tensor of the form given by Eq. (2.4), which corresponds to a perfect fluid as the matter content. The barotropic equation of state is expressed by Eq. (2.8), while a spatially flat geometry ($k=0$) is assumed. The model delineates three distinct epochs, each characterized by different types of fluid domination and distinct values of the coupling parameter ω, reflecting the key phases in the Universe's evolution.

To demonstrate how the effects of a general scalar-tensor theory at any given moment can be reduced to those of a Jordan-Brans-Dicke (JBD) theory, we develop the field equations for scalar-tensor theories (Eqs. (4.8)-(4.9)), allowing the coupling parameter ω to vary with the scalar field ϕ. To facilitate this, we introduce the conformal time η defined through the differential relation

$$dt=ad\eta, \tag{4.11}$$

along with the variables defined in [179]

$$X\equiv\phi a^2, \quad Y\equiv\int\sqrt{\frac{2\omega+3}{3}}\frac{\mathrm{d}\phi}{\phi}, \tag{4.12}$$

and the relation between $\rho(t)$ and $a(t)$

$$\rho(t)=\rho_0\left(\frac{a}{a_0}\right)^{-3\gamma}, \tag{4.13}$$

which is obtained by integrating the energy conservation equation (Eq. (2.7)) using the barotropic equation of state (Eq. (2.8)). The field equations (4.8)-(4.10) can thus be rewritten as

$$(X')^2+4kX^2-(Y'X)^2=4MX\left(\frac{X}{\phi}\right)^{\frac{4-3\gamma}{2}}, \tag{4.14}$$

$$X''+4kX=3M(2-\gamma)\left(\frac{X}{\phi}\right)^{\frac{4-3\gamma}{2}}, \tag{4.15}$$

$$(Y'X)'=M(4-3\gamma)\sqrt{\frac{3}{2\omega+3}}\left(\frac{X}{\phi}\right)^{\frac{4-3\gamma}{2}}, \tag{4.16}$$

where the prime denotes differentiation with respect to η and $M\equiv 8\pi\rho_0/3$, with ρ_0 being an arbitrary initial condition for the energy density. Two key aspects of the scalar-tensor cosmological solutions are critical for understanding the interaction between quantum processes and the Universe's expansion during epochs relevant to baryogenesis. First, these processes occur during the radiation epoch, where the early expansion is dominated by the scalar field's energy density [176, 179]. Second, Eq. (4.12), valid during the radiation epoch, allows the definition of an average value of the coupling parameter, $\langle\omega\rangle$, over any time interval, even if ω is strictly increasing. Specifically, for any time interval $[t_i, t_j]$, we define

$$\sqrt{\frac{2\langle\omega\rangle_{ij}+3}{3}} = \frac{\int_{t_i}^{t_j}\sqrt{\frac{2\omega+3}{3}}\frac{\mathrm{d}\phi}{\phi}}{\int_{t_i}^{t_j}\frac{\mathrm{d}\phi}{\phi}}, \tag{4.17}$$

enabling the treatment of a general scalar-tensor theory as a Brans-Dicke theory with a constant coupling $\langle\omega\rangle_{ij}$, averaged over the given time interval.

We divide the radiation epoch into two intervals: the first corresponds to a stage dominated by the Jordan-Brans-Dicke (JBD) scalar field, while the second is characterized by radiation and ultra-relativistic matter domination over the scalar field. This phase is followed by a matter-dominated era, where $p \sim 0$. The full evolution is described by the following three-epoch solution for a flat FLRW Universe in the general JBD framework

$$0 \le t \le t_c: \quad a(t) = A_1 t^q, \tag{4.18}$$

$$t_c \le t \le t_{eq}: \quad a(t) = A_2 (t - t_{20})^{1/2}, \tag{4.19}$$

$$t_{eq} \le t \le t_0: \quad a(t) = A_3 (t - t_{30})^{\frac{2\omega+2}{3\omega+4}}, \tag{4.20}$$

where q is given by [180] as

$$q \equiv \frac{\omega}{3\left(\omega + 1 \mp \sqrt{\frac{2\omega+3}{3}}\right)}, \tag{4.21}$$

and A_1, A_2, A_3, t_{20}, and t_{30} are constants, determined by the junction conditions that ensure the smoothness of the solution. Continuity of both the scale factor and its first derivative at $t = t_c$ and $t = t_{eq}$ leads to the following relations

$$A_2 = \sqrt{2q} A_1 t_c^{q-1/2}, \tag{4.22}$$

$$t_{20} = \left(1 - \frac{1}{2q}\right) t_c, \tag{4.23}$$

and

$$A_3 = \sqrt{2q} A_1 t_c^{q-1/2} \left(\frac{4\omega+4}{3\omega+4}\right)^{-\frac{2\omega+2}{3\omega+4}} (t_{eq} - t_{20})^{\frac{1}{2} - \frac{2\omega+2}{3\omega+4}}, \tag{4.24}$$

$$t_{30} = -\frac{\omega}{3\omega+4} t_{eq} + t_{20}. \tag{4.25}$$

In this solution, the Brans-Dicke scalar field evolves as

$$0 \le t \le t_c: \quad \phi(t) = \phi_1 t^{\frac{1-3q}{3}}, \tag{4.26}$$

$$t_c \le t \le t_{eq}: \quad \phi(t) = \phi_2, \tag{4.27}$$

$$t_{eq} \le t \le t_0: \quad \phi(t) = \phi_3 (t - t_{30})^{\frac{2}{3\omega+4}}, \tag{4.28}$$

where ϕ_1, ϕ_2, and ϕ_3 are constants that ensure the continuity of ϕ at t_c and t_{eq}.

In the first epoch, for $0 \le t \le t_c$, the sign of $\dot{\phi}/\phi$ depends on q. For $q > 1/3$, which corresponds to the $(-)$ branch in Eq. (4.21) (denoted q_-), we find that $\dot{\phi}/\phi$ is negative, leading to a decreasing ϕ

and consequently a gravitational constant G that increases towards infinity over time. In cases where $q > 1$, corresponding to the $(+)$ branch (denoted q_+), this leads to accelerated expansion, and occurs for $-3/2 \leq \omega < -4/3$. Conversely, for $q < 1/3$, which is always associated with the $(+)$ sign, $\dot{\phi}/\phi$ is positive, implying that ϕ increases with time, causing G to approach zero as $t \to \infty$. It is also worth noting that for $q < 0$, corresponding to $-4/3 < \omega < 0$, the scale factor contracts with time.

4.1.2 STT and inflation

Since the early development of the inflationary paradigm, scalar-tensor theories have played a pivotal role. A notable early contribution was the proposal of Extended Inflation [181], where inflation was first linked to alternative theories of gravity. This model revived the spirit of Guth's original inflationary concept, proposing a first-order phase transition associated with high-energy particle physics. However, unlike standard inflation driven by General Relativity (GR), Extended Inflation employed a Jordan-Brans-Dicke (JBD) framework. In this setup, the expansion of the universe was driven by a vacuum energy, leading to a rapid power-law expansion instead of the exponential one predicted by GR. The model incorporated a Higgs-like sector within the matter Lagrangian, undergoing a strongly first-order phase transition. A key implication of this approach is that ε, which remains constant in other models (since H depends on false vacuum energy and λ on the barrier shape), becomes time-dependent. By allowing the Newtonian gravitational constant to decrease during inflation, the expansion rate could also decrease, leading to a growing ε, potentially crossing a critical threshold ε_{cr}.

Building on this work, Steinhardt and Accetta (1991) introduced a more sophisticated model, termed "hyperextended inflation" [182], designed to overcome some of the challenges associated with extended inflation. They adopted a more general scalar-tensor framework, formulating the Lagrangian as follows [183]

$$\mathcal{L}_\phi = f(\phi)R - \frac{1}{2}\partial_\mu\phi\,\partial^\mu\phi - \frac{1}{2}\partial_\mu\sigma\,\partial^\mu\sigma - V(\sigma) + 16\pi\mathcal{L}_{\text{other}}\,, \tag{4.29}$$

where $f(\phi)$ is the non-minimal coupling between the scalar field ϕ and the curvature R, and $\mathcal{L}_{\text{other}}$ represents the Lagrangian of the matter fields other than the inflaton.

Similar to extended inflation, hyperextended inflation follows the old inflationary scenario, with the scalar field σ trapped in a false vacuum state. The false vacuum energy density $V(\sigma)$ dominates, driving superluminal expansion. Inflation ends when quantum tunneling nucleates bubbles of true vacuum, which expand near the speed of light. In this model, the effective Newton's constant is inversely proportional to $f(\phi)$, meaning that if $f(\phi)$ increases, the effective gravitational constant decreases, leading to a decrease in H and ε. Almost any monotonically increasing $f(\phi)$ can be utilized during inflation [182]. By redefining the field as $\phi = f(\phi)$, the Lagrangian simplifies to

$$\mathcal{L}_\phi = \phi R - \frac{\omega(\phi)}{\phi}\partial_\mu\phi\,\partial^\mu\phi - \frac{1}{2}\partial_\mu\sigma\,\partial^\mu\sigma - V(\sigma) + 16\pi\mathcal{L}_{\text{other}}\,, \tag{4.30}$$

where $\omega(\phi) = f(\phi)/(2f'(\phi))$. This Lagrangian leads to an action that is entirely equivalent to the action in (4.2) when $\lambda(\phi)$ vanishes and $\mathcal{L}_M = \mathcal{L}_{\text{other}} + \mathcal{L}_\sigma$. In particular, for the case of $f(\phi) = \xi\phi^2$, where ξ is a constant, the result is $\omega = \xi/8$, a constant, thereby recovering the standard Jordan-Brans-Dicke (JBD) framework and, within it, the results of extended inflation. From this, one can see that the basic idea behind hyperextended inflation closely follows the principles of extended inflation. However, if one considers a more complex form like $f(\phi) = \xi(\phi^2 + \phi^{n+2}/M^n)$, where $n > 2$ and ξ is a constant (as in [182]), some intriguing consequences emerge. In this model, for $\phi \gg M$, the behavior of extended inflation is recovered. However, as ϕ approaches the order of M, the inclusion of higher-order nonminimal couplings slows down the cosmic expansion even further. This could result in a wider range of initial conditions and parameters that allow for an acceptable distribution of bubble sizes (see, for example, [184]). Despite this, by the end of inflation, ω should approach $\mathscr{O}(1)$. Interestingly, as the higher-order terms in $f(\phi)$ become more significant, $f(\phi)$ could reach a maximum value at some point beyond the end of inflation. As a result, $f'(\phi)$ would tend toward zero, causing $\omega(\phi) = f(\phi)/(2f'(\phi))$ to approach infinity, which would halt the evolution of ϕ. At this stage, the model would become indistinguishable from GR. It is worth noting that Barrow and Maeda [185] used the Lagrangian (4.30) and treated $\omega(\phi)$ as their fundamental expression, expanding it in a truncated Taylor series as $\omega(\phi) = \omega_0 + \omega_m \phi^m$ for some m. While the Lagrangians in (4.29) and (4.30) are equivalent, choosing $\omega(\phi)$ as the simplest function rather than $f(\phi)$ leads to the construction of distinct models. In fact, when $f(\phi)$ contains more than two terms, it is generally impossible to express the equivalent $\omega(\phi)$ in closed form because one would need $\phi = f^{-1}(\phi)$, and f may not be analytically invertible. Additionally, Steinhardt and Accetta's approach introduces a singularity in the ϕ-ϕ transformation for certain values of ϕ, meaning that there is no analytic $\omega(\phi)$ corresponding to their formulation. These approaches have been extensively discussed in [186].

Despite the appeal of hyperextended inflation, it appears difficult to implement it successfully when all observational constraints are considered. As noted in [187], for models of this type, where bubble nucleation ends inflation, there is no way to reconcile all observational constraints and achieve a viable inflationary scenario.

4.2 $f(R,\mathcal{T}^2)$ gravity

The modified theory of gravity $f(R,\mathcal{T}^2)$ [188] was initially developed to address the late-time acceleration problem, but it also showed promising results in tackling issues related to spacetime singularities [189, 190] that occur within the framework of GR. Since GR alone is insufficient due to the anticipated effects of quantum gravity.

The action for $f(R,\mathcal{T}^2)$ gravity reads [188]

$$S = \frac{1}{2\kappa}\int \mathrm{d}^4x\sqrt{-g}f(R,\mathcal{T}^2) + \int \mathrm{d}^4x\sqrt{-g}\mathcal{L}_m\,, \tag{4.31}$$

where $\kappa = 8\pi G = M_{Pl}^{-2}$ and $f(R,\mathcal{T}^2)$ is a well behaved function of the Ricci scalar and $\mathcal{T}^2$ and $\mathcal{L}_m$ is the matter Lagrangian. Varying the action with respect to the inverse metric, we find [190]

$$\delta S = \frac{1}{2\kappa}\int_{\mathcal{M}} \{f_R \delta R + f_{\mathcal{T}^2}\delta(T_{\mu\nu}T^{\mu\nu}) - \frac{1}{2}g_{\mu\nu} f \delta g^{\mu\nu} + \frac{1}{\sqrt{-g}}\delta(\sqrt{-g}\mathcal{L}_m)\}\mathrm{d}^4x, \tag{4.32}$$

where subscripts denote differentiation with respect to R and $\mathcal{T}^2$, respectively. We define

$$\theta_{\mu\nu} \equiv \frac{\delta(T_{\alpha\beta}T^{\alpha\beta})}{\delta g^{\mu\nu}} = -2L_m(T_{\mu\nu} - \frac{1}{2}g_{\mu\nu}T) - TT_{\mu\nu} + 2T^{\alpha}_{\mu}T_{\nu\alpha} - 4T^{\alpha\beta}\frac{\partial^2 L_m}{\partial g^{\mu\nu}\partial g^{\alpha\beta}}\,, \tag{4.33}$$

From Eq.(4.32) we obtain the field equations

$$f_R R_{\mu\nu} - \frac{1}{2} f g_{\mu\nu} + (g_{\mu\nu}\nabla_\alpha\nabla^\alpha - \nabla_\mu\nabla_\nu) f_R = \kappa(T_{\mu\nu} - \frac{1}{\kappa} f_{\mathcal{T}^2}\theta_{\mu\nu}). \tag{4.34}$$

These reduce, as expected, to the field equations for $f(R)$ gravity in the special case where $f(R,\mathcal{T}^2) =$

$f(R)$ (see [191] for a complete review of this theory) and to the Einstein equations without a cosmological constant when $f(R,\mathcal{T}^2)=R$. Assuming a perfect fluid for $T_{\mu\nu}$, Eq.(2.4), and $\mathcal{L}=p$ [192] we have

$$T=3p-\rho \quad , \quad \mathcal{T}^2=\rho^2+3p^2 \tag{4.35}$$

and

$$\theta_{\mu\nu}=-(\rho^2+4p\rho+3p^2)u_\mu u_\nu\,. \tag{4.36}$$

In the context of $f(R,\mathcal{T}^2)$ gravity, we examine a particular class of models characterized by the form [146]

$$f(R,\mathcal{T}^2)=R+\eta M_{Pl}^{2-8n}\left(\mathcal{T}^2\right)^n, \tag{4.37}$$

which is referred to as energy-momentum powered gravity. This model represents a specific case of $f(R,\mathcal{T}^2)$ theories. In this formulation, η is a dimensionless constant that determines the coupling strength associated with the scalar $\mathcal{T}^2$, while the parameter n governs the specific form of the model. The inclusion of the term M_{Pl}^{2-8n} ensures the proper dimensional consistency of the new terms introduced by $\mathcal{T}^2$ in the cosmological equations. For convenience, we define a new constant, $\eta'=\eta M_{Pl}^{2-8n}$. When $n=1$, the model was studied in [189], and the cases $n=1/2$ and $n=1/4$ correspond to models that have been studied in [188].

For this model, the field equations reduce to

$$R_{\mu\nu}-\frac{1}{2}g_{\mu\nu}R=\kappa T^{\text{eff}}_{\mu\nu}, \tag{4.38}$$

where $T^{\text{eff}}_{\mu\nu}$ is given by

$$T^{\text{eff}}_{\mu\nu}=T_{\mu\nu}+\frac{\eta'}{\kappa}(\mathcal{T}^2)^{n-1}\left[\frac{1}{2}(\mathcal{T}^2)g_{\mu\nu}-n\theta_{\mu\nu}\right]. \tag{4.39}$$

Taking the trace of the field equations one obtains

$$2\left(\mathcal{T}^2\right)^n-n\left(\mathcal{T}^2\right)^{n-1}\theta=-\frac{1}{\eta'}\left(\kappa T+R\right), \tag{4.40}$$

with θ being the trace of $\theta_{\mu\nu}$ and T the trace of the energy-momentum tensor. This equation allows us to evaluate $\mathcal{T}^2$ depending on the choice of n.

4.2.1 Cosmology in $f(R,\mathcal{T}^2)$ gravity

Using the FLRW metric and the field equations (4.38), one obtains the following modified Friedmann equations [190]

$$H^2=\kappa\frac{\rho}{3}+\frac{\eta'}{3}(\rho^2+3p^2)^{n-1}\left[(n-\frac{1}{2})(\rho^2+3p^2)+4n\rho p\right], \tag{4.41}$$

$$\dot{H}+H^2=-\kappa\frac{\rho+3p}{6}-\frac{\eta'}{3}(\rho^2+3p^2)^{n-1}\left[\frac{n+1}{2}(\rho^2+3p^2)+2n\rho p\right], \tag{4.42}$$

where $H\equiv\dot{a}/a$ is the Hubble parameter. Considering now the barotropic equation of state, $p=w\rho$, the previous equations can be recast as [146, 190]

$$H^2=\kappa\frac{\rho}{3}+\frac{\eta'\rho^{2n}}{3}C_{Frd}(n,w), \tag{4.43}$$

where C_{Frd} is a function that depends on the choice of n and w given by

$$C_{Frd}(n,w) \equiv (1+3w^2)^{n-1}\left[(n-\frac{1}{2})(1+3w^2)+4nw\right], \tag{4.44}$$

and the acceleration equation reduces to [146, 190]

$$\dot{H}+H^2 = -\kappa\frac{1+3w}{6}\rho - \frac{\eta'\rho^{2n}}{3}C_{Acc}(n,w), \tag{4.45}$$

where C_{Acc} returns a constant based on the choice for n and w, and is given by

$$C_{Acc} \equiv (1+3w^2)^{n-1}\left[\frac{n+1}{2}(1+3w^2)+2nw\right]. \tag{4.46}$$

A notable aspect of this modified theory of gravity is the presence of the ρ^{2n} term in both equations, which bears a resemblance to quantum geometric effects observed in loop quantum gravity [193] and braneworld scenarios [194]. Finally, the modified continuity equation is obtained by direct derivation from the Friedmann equation (4.41) leading to [146, 190]

$$\dot{\rho} = -3H\rho(1+w)C_{con}(n,w), \tag{4.47}$$

where $C_{con}(n,w)$ is the extra term originated from $\mathcal{T}^2$, and is given by

$$C_{con}(n,w) \equiv \left[\frac{\kappa+\eta'\rho^{2n-1}n(1+3w)(1+3w^2)^{n-1}}{\kappa+2\eta'\rho^{2n-1}nC_{Frd}(n,w)}\right]. \tag{4.48}$$

A detailed examination of the cosmological equations shows that the overall cosmological behavior is primarily governed by the three functions under consideration ($C_{Frd}(n,w)$, $C_{Acc}(n,w)$ and $C_{con}(n,w)$), along with the specific value of n chosen. In the context of baryogenesis, we concentrate on the radiation-dominated era that follows inflation, thereby circumventing the problem of symmetry washout caused by inflation. In this epoch, it is standard to set $w = 1/3$, as this equation of state corresponds to a radiation-dominated universe. Nevertheless, it is important to note that, with this assumption, Eq. (4.47) does not simplify to the usual form for the energy density, $\rho \propto a^{-4}$, as typically expected for the radiation era. To address this issue, one can impose the condition

$$C_{con}(n,w) = 1, \tag{4.49}$$

as proposed in [190]. While this condition successfully reproduces the standard GR continuity equation, it imposes unnecessary restrictions on the parameters n and w. Instead, if the aim is merely to recover the familiar form of the energy density for a radiation-dominated universe, a less stringent condition can be employed by imposing

$$(1+w)C_{con}(n,w) = \frac{4}{3}. \tag{4.50}$$

Solving this constraint for ρ^{2n-1} leads to the expression

$$\rho^{2n-1} = \frac{1-3w}{\eta M_{Pl}^{4-8n}\left(3nA(w)-8nC_{Frd}\right)}, \tag{4.51}$$

where $A(w)$ is defined as

$$A(w) \equiv (1+w)(1+3w)(1+3w^2)^{n-1}\,. \tag{4.52}$$

Upon analyzing Eq.(4.51), it becomes evident that the right-hand side corresponds to a constant. For the equation to yield a physically meaningful solution within a dynamical cosmological setting, it is necessary to set $n = 1/2$, as a constant ρ would not be viable. This result highlights the significance of the $n = 1/2$ model within energy-momentum powered gravity, as it successfully reproduces the form $\rho \propto a^{-4}$ for specific values of η and w. By imposing $n = 1/2$, the condition (4.51) can be reformulated to establish a relation between η and w, resulting in

$$\eta_* \equiv \eta(w) = \frac{1-3w}{\frac{3}{2}A(w) - 4C_{Frd}(\frac{1}{2}, w)}\,. \tag{4.53}$$

This relationship not only ensures the correct form of the energy density, but also serves as a constraint on η. The value of w dictates the η necessary to satisfy this condition, opening up new possibilities to investigate baryogenesis. An intriguing result is that for $w = 1/3$, the required η becomes zero, effectively reducing the theory to GR. This result will be explored in further detail in the subsequent section.

Chapter 5

Baryogenesis in Modified gravity

In this chapter, the results for **Path A** and **Path B** will be presented. The results for the EWB and GUTB are from [116] and the GB results from [146].

5.1 Scalar-Tensor EWB

A distinct thermal history of the Universe can significantly affect Electroweak Baryogenesis (EWB). This consideration arises from the sphaleron bound, a critical criterion which, if unmet by a specific EWB model, invalidates it as a viable explanation for the observed baryon asymmetry of the Universe (BAU).

The sphaleron bound is derived based on a particular assumption regarding the expansion rate of the Universe, and it can be relaxed if an alternative thermal history is considered. In the context of scalar-tensor theories, this bound must be reformulated in terms of the expansion rate during the early cosmological epochs. However, due to its similarity with GR, the second epoch is not expected to substantially alter the sphaleron bound. Moreover, as the third epoch occurs much later than the relevant timeframe, we focus on expressing the expansion rate for the first two epochs in STT in terms of both the temperature and the expansion rate for a radiation-dominated Universe in standard cosmology (H), as follows

$$\begin{aligned} \Gamma_{e_1}(T) &= \frac{H(T)}{\zeta}\left(\frac{T_c}{T}\right)^{\frac{2q-1}{q}}, \qquad && T \geq T_c, \\ \Gamma_{e_2}(T) &= \frac{H(T)}{\zeta}, && T_c \geq T \geq T_{eq}, \end{aligned} \tag{5.1}$$

where $H(T) = 1.66\sqrt{g_*}T^2/M_{Pl}$ and ζ is defined as [177, 179]

$$\zeta = \left[\left(\frac{\rho_0^R}{\rho_0^M}\right)^{\frac{1}{2\omega+2}}\right], \tag{5.2}$$

with ρ_0^R and ρ_0^M representing the present-day radiation and matter energy densities, respectively.

Consequently, the sphaleron bound from Eq. (3.17) can be reformulated for STT as

$$\sqrt{\frac{4\pi}{\alpha_W}}\frac{\phi_{Cr}}{T_{Cr}}B-7\ln\left(\sqrt{\frac{4\pi}{\alpha_W}}\frac{\phi_{Cr}}{T_{Cr}}B\right)\gtrsim \begin{cases}\ln\left[\frac{2.8\times10^5\kappa\mathcal{M}}{5\ln 10\;B^7}\left(\frac{\alpha_w}{4\pi}\right)^4\right]+\ln\left(\frac{T_{Cr}}{2H_{Cr}}\right)+\left(\frac{2q-1}{q}\right)\ln\left(\frac{T_{Cr}}{T_c}\right)+\ln(\zeta), & T_{Cr}\geq T_c,\\ \ln\left[\frac{2.8\times10^5\kappa\mathcal{M}}{5\ln 10\;B^7}\left(\frac{\alpha_w}{4\pi}\right)^4\right]+\ln\left(\frac{T_{Cr}}{2H_{Cr}}\right)+\ln(\zeta), & T_{Cr}\leq T_c.\end{cases} \tag{5.3}$$

It follows that, to significantly relax the sphaleron bound, the phase transition must occur during the first epoch. From Eq.(5.1), it is clear that the parameter q must be smaller than $1/2$; otherwise, the expansion rate during the first epoch will negatively impact the sphaleron bound by raising its lower limit instead of lowering it. This is because, for $q>1/2$, the expansion rate in the first cosmological epoch in STT is lower than the standard GR expansion rate for a radiation-dominated Universe, making the sphaleron processes in the broken phase more effective in erasing the asymmetry.

In addition to the requirement of a strong first-order phase transition, another critical condition must be satisfied to ensure efficient baryon number violation. Specifically, sphalerons must be in equilibrium during the symmetric phase. This can be achieved by ensuring that the rate of baryon number non-conserving processes in the broken phase exceeds the expansion rate of the Universe. Utilizing the thermal rate per unit volume of sphaleron events, as given by Eq.(3.4), the rate of baryon number non-conserving processes in the symmetric phase can be expressed as

$$V_B^{\text{sym}}=\frac{\mathcal{M}}{T^3}\Gamma_{\text{sph}}^{\text{sym}}=\mathcal{M}\kappa\alpha_W^4 T\ . \tag{5.4}$$

With this result, the rate of baryon number non-conserving processes in the symmetric phase can be explicitly written as

$$V_B^{\text{sym}}=25\mathcal{M}\alpha_W^5 T\ . \tag{5.5}$$

Thus, under the standard cosmological scenario, the condition for sphaleron transitions to be in equilibrium during the symmetric phase is given by

$$V_B^{\text{sym}}(T)>H(T)\quad\Leftrightarrow\quad T<7.53\mathcal{M}\alpha_W^5\frac{m_{Pl}}{\sqrt{g_*}}\ . \tag{5.6}$$

It is useful to define the temperature T_{GR}^{sph} at which sphaleron transitions enter equilibrium, expressed as

$$T_{GR}^{\text{sph}}\equiv 7.53\mathcal{M}\alpha_W^5\frac{m_{Pl}}{\sqrt{g_*}}\ , \tag{5.7}$$

where T_{GR}^{sph} represents the temperature for sphaleron equilibrium in the context of General Relativity corresponding to $T_{GR}^{\text{sph}}\simeq 7.5\times10^{12}$ GeV. Similarly, for the first cosmological epoch in STT, the condition for sphaleron equilibrium in the symmetric phase can be written as

$$V_B^{\text{sym}}(T)>\Gamma_{e_1}(T)\quad\Leftrightarrow\quad T<T_c\left(\frac{T_{GR}^{\text{sph}}}{T_c}\zeta\right)^{\pm\left|\frac{q}{1-q}\right|}\ , \tag{5.8}$$

where the negative sign corresponds to $q<0$ or $q>1$, and the positive sign applies to $0<q<1$. Similarly, the temperature $T_{STT}^{\rm sph}$, which marks the crossover between $V_B^{\rm sym}(T)$ and $\Gamma_{e_1}(T)$, is defined as

$$T_{STT}^{\rm sph} \equiv T_c \left(\frac{T_{GR}^{\rm sph}}{T_c} \zeta \right)^{\pm \left| \frac{q}{1-q} \right|} . \tag{5.9}$$

To ensure clarity, let us impose that the phase transition occurs after sphaleron processes have reached equilibrium in the symmetric phase, and that nucleosynthesis takes place during the second epoch following the phase transition. This leads to three possible hypotheses concerning the sequence of these events:

1. The sphaleron processes enter in equilibrium in the symmetric phase before the phase transition and the phase transition occurs before the transition for the second epoch, which occurs before nucleosynthesis.
2. The sphaleron processes enter in equilibrium in the symmetric phase before the transition for the second epoch and the phase transition occurs in the second epoch before the nucleosynthesis.
3. The transition for the second epoch happens before the sphaleron processes reach the equilibrium. Then, sphaleron processes enter in equilibrium in the symmetric phase before the phase transition, which happens before nucleosynthesis.

Analyzing these three events, one can rationalize that the first hypothesis is the one most relevant for the EWB because, as stated before, the first epoch presents the most impact ruling out the second hypothesis and third hypothesis. In terms of temperature relations, the first hypothesis is expressed a

$$T_{GR}^{sph} > \theta_2^{-1} T_{Cr}^{\frac{1-q}{q}} T_c^{\frac{2q-1}{q}} > \theta_2^{-1} T_c > \theta_2^{-1} T_N^{\frac{1-q}{q}} T_c^{\frac{2q-1}{q}} \quad \text{if} \quad 0 < q < 1 , \tag{5.10}$$

that by using the constraint $q < 1/2$ can be recast as

$$\frac{1}{2} > q > \ln T_c \left[\ln \left(\frac{T_c^2}{\zeta} \frac{T_{Cr}}{T_{GR}^{sph}} \right) \right]^{-1} \qquad \wedge \qquad T_c > \left(\frac{T_{GR}^{sph} \zeta}{T_{CR}} \right)^{\frac{q}{2q-1}} T_{Cr} \wedge T_c > T_N . \tag{5.11}$$

The simultaneous satisfaction of the two latter conditions related with the temperature is necessary because for

$$q > \ln(T_N/T_{Cr})/\ln[T_N^2/(T_{GR}^{sph}\zeta)] \simeq 0.2 , \tag{5.12}$$

we get

$$\left(T_{GR}^{sph} \zeta / T_{CR} \right)^{q/(2q-1)} T_{Cr} < T_N . \tag{5.13}$$

The intersection of conditions can be written as two conditions for two different ranges of q. However, numerically, the expression presented in Eq. (5.11) is easier to compute.

To conclude this brief analysis, it is important to understand that the condition (5.11) is a necessary condition for a viable electroweak baryogenesis scenario to take place during the first STT cosmological epoch. Additionally, an important notation to have is related with the ability to constraint the new parameters of Eq.(5.3). The main way to do it is to use the Big-Bang nucleosynthesis data. To do such, one can compute the ratio between the STT expansion rate and GR expansion rate in terms of temperature creating a relation between these two theories that differ by the term ζ [177, 178] that can be constrained by the BNN data.

5.2 Scalar-Tensor GUTB

Following the framework defined in 3.4, it will be employed the STT outcomes to see if GUTB can be positively affect by modifications to gravity. Moreover, the mechanism proposed should be regarded as a preliminary approximation to more realistic GUT scenarios [96]. Taking this into account, the Boltzmann equations governing the evolution of baryon asymmetry in the model are expressed as follows

$$\dot{X} = -\Gamma_D (X - X_{EQ}), \tag{5.14}$$

$$\dot{B} = \varepsilon \Gamma_D (X - X_{EQ}) - (\Gamma_{ID} + 2\Gamma_S) B, \tag{5.15}$$

with B being the Baryon number per comoving volume and X being the number of X's per comoving volume where

$$X = 8\, g_{*a} N_X X = 8\, g_{*a} N_{X_{EQ}} B = 8\, g_{*a} \varepsilon N_B \,, \tag{5.16}$$

where g_{*a} represents the degrees of freedom for radiation during the relevant epoch, ε characterizes the extent of CP violation, N_X denotes the number density of a generic self-conjugate supermassive boson, and $N_{X_{EQ}}$ is its equilibrium number density. Additionally,

$$N_B = \frac{N_b - N_{\bar{b}}}{2} \,, \tag{5.17}$$

defines the net baryon number, while Γ_j, with $j = D, ID, S$, refers to the decay rate of the supermassive boson X, its inverse decay rate, and the rate of baryon-number-violating (BNV) scattering, respectively.

In order to proceed, it is useful to introduce a new dimensionless, dynamical variable defined by $\bar{z} = m_X/T$, where m_X is the mass of the generic supermassive boson X. In terms of this variable, the rescaled equilibrium number of supermassive bosons X is given by

$$X_{EQ} = 2a(\bar{z}) \,, \tag{5.18}$$

where

$$a(\bar{z}) \equiv \frac{\bar{z}^2}{2} K_2(\bar{z}) \simeq \begin{cases} 1 & \text{if } \bar{z} \ll 1 \\ \frac{1}{2}\sqrt{\frac{\pi}{2}}\bar{z}^{3/2} \exp(-\bar{z}) & \text{if } \bar{z} \gg 1 \end{cases} \,, \tag{5.19}$$

and $K_2(\bar{z})$ is the modified Bessel function of the second kind. The thermal expansion rate of the Universe during the first and second epochs can be expressed as

$$\Gamma_{e_i}(\bar{z}) = \begin{cases} \Gamma_{e_1}(T) = \frac{\sqrt{g_*}}{0.602 m_{Pl_0}} \frac{m_X^2}{\zeta} \left(\frac{\bar{z}_c}{\bar{z}}\right)^{1/q-2} \bar{z}^{-2} \,, & \text{if } 0 \leq \bar{z} \leq \bar{z}_c \\ \Gamma_{e_2}(T) = \frac{\sqrt{g_*}}{0.602 m_{Pl_0}} \frac{m_X^2}{\zeta} \bar{z}^{-2} \,, & \text{if } \bar{z}_c \leq \bar{z} \leq \bar{z}_{eq} \end{cases} \,, \tag{5.20}$$

where $i = 1,\ 2$ denote the first and second radiation-dominated epochs, and $\bar{z}_c = T_c/m_X$, $\bar{z}_{eq} = T_{eq}/m_X$ represent the values of $\bar{z}$ corresponding to the transition to the second epoch and the time of matter-radiation equality, respectively. Additionally, the following differential relation holds

$$\mathrm{d}t = \frac{\mathrm{d}\bar{z}}{\bar{z}\Gamma_{e_i}(\bar{z})} \,. \tag{5.21}$$

Analogously to what has been done in GR, it is useful to define the quantity

$$K_{STT_i} \equiv \left(\frac{\Gamma_D}{\Gamma_{e_i}}\right)_{\bar{z}=1} = \begin{cases} K_{STT_1} = K_{GR}\,\zeta\,\bar{z}_c^{\frac{2q-1}{q}} & \text{if } 0 \leq \bar{z} \leq \bar{z}_c \\ K_{STT_2} = K_{GR}\,\zeta & \text{if } \bar{z}_c \leq \bar{z} \leq \bar{z}_{eq} \end{cases}, \tag{5.22}$$

which measures the effectiveness of decays at the critical epoch $\bar{z} = 1$ ($m_X = T$), when the number of self-conjugate supermassive bosons X must decrease to maintain equilibrium. By substituting Eq. (5.22) into the differential relation in Eq. (5.21), we obtain

$$\mathrm{d}t = \frac{K_{STT_i}}{\Gamma_D(\bar{z}=1)} f_i(\bar{z})\,\mathrm{d}\bar{z}, \tag{5.23}$$

where

$$f_i(\bar{z}) \equiv \bar{z}^{-1}\frac{\Gamma_{e_i}(\bar{z}=1)}{\Gamma_{e_i}(\bar{z})} = \begin{cases} f_1(\bar{z}) = \bar{z}^{\frac{1-q}{q}} & \text{if } 0 \leq \bar{z} \leq \bar{z}_c \\ f_2(\bar{z}) = \bar{z} & \text{if } \bar{z}_c \leq \bar{z} \leq \bar{z}_{eq} \end{cases}. \tag{5.24}$$

The substitution of this relation and the rescaled equilibrium number of bosons X from Eq. (5.18) into the Boltzmann equations (5.14)-(5.15), corresponding to a change of variable, yields

$$X' = -K_{STT_i} f_i\left[\gamma_D\,(X-2a) + \gamma_A\,(X^2-4a^2)\right], \tag{5.25}$$

$$B' = K_{STT_i} f_i\left[\varepsilon\gamma_D\,(X-2a) - (\gamma_{ID}+\gamma_S)\,B\right], \tag{5.26}$$

where the prime $'$ denotes differentiation with respect to $\bar{z}$, and $\gamma_j \equiv \Gamma_j(\bar{z})/\Gamma_D(\bar{z}=1)$, such that

$$\gamma_D = \frac{\sqrt{2}}{\sqrt{\bar{z}^{-2}+1}} \simeq \begin{cases} \bar{z} & \text{if } \bar{z} \lesssim 1 \\ 1 & \text{if } \bar{z} \gtrsim 1 \end{cases}, \tag{5.27}$$

$$\gamma_{ID} = 2\frac{a(\bar{z})}{\sqrt{\bar{z}^{-1}+1}} \simeq \begin{cases} 2\bar{z} & \text{if } \bar{z} \lesssim 1 \\ \sqrt{\frac{\pi}{2}}\bar{z}^{3/2}\exp(-\bar{z}) & \text{if } \bar{z} \gtrsim 1 \end{cases}, \tag{5.28}$$

$$\gamma_S = \frac{A\alpha_X}{\bar{z}(1+\bar{z}^2)^2} \simeq \begin{cases} A\alpha_X\bar{z}^{-1} & \text{if } \bar{z} \lesssim 1 \\ \frac{A\alpha_X}{\bar{z}^5} & \text{if } \bar{z} \gtrsim 1 \end{cases}, \tag{5.29}$$

$$\gamma_A \simeq \begin{cases} \frac{\alpha_X^2}{\alpha_H}\bar{z}^{-1} & \text{if } \bar{z} \lesssim 1 \\ \frac{\alpha_X^2}{\alpha_H}\bar{z}^{-3} & \text{if } \bar{z} \gtrsim 1 \end{cases}, \tag{5.30}$$

where A is a numerical factor introduced to account for more realistic GUT characteristics, such as the number of scattering channels. The freeze-out condition $\Gamma_{e_i}(\bar{z}_{f_{ji}}) \simeq \Gamma_j(\bar{z}_{f_{ji}})$, where $\bar{z}_{f_{ji}}$ is the value of $\bar{z}$ at which the j-process freezes during epoch i, can be expressed as

$$f_i(\bar{z}_{f_{ji}}) = K_{STT_i}\gamma_j(\bar{z}_{f_{ji}})\,. \tag{5.31}$$

From Eq. (5.22), it is evident that the parameter K_{STT_i} reflects the modification's impact on the expansion rate, and consequently, the time-temperature relation, in the STT toy model. This is further illustrated in the Boltzmann equations (5.26). The differences between STT and GR that influence baryon asymmetry generation primarily arise during the first epoch, dominated by the Jordan-Brans-Dicke (JBD) scalar field. The impact is once again mainly encoded in the q parameter. Additionally, the four processes that can occur during the asymmetry production also are affected by the STT theory and a careful examination is necessary. Furthermore, at a first-glance the BBN data also can constraint the parameter z_c as the temperature T_c cannot be truly a free parameter as it would had implications in the

BNN and also the mass of X follows this logic.

5.3 Gravitational Baryogenesis in $f(R,\mathcal{T}^2)$ gravity

When employing modifications to gravity in the context of gravitational baryogenesis a key component arises. Besides the usual term (3.26), it is possible and rationale to consider another terms that instead of using the Ricci scalar. This new terms are linked to the specific modified theory of gravity being utilized and are introduced in a similar manner to spontaneous baryogenesis, in other words, one can consider

$$\mathcal{L}_{int} = \frac{1}{M_*^2}\,\partial_\mu(R)J_B^\mu \xrightarrow{\text{Modified Gravity}} \mathcal{L}_{int} = \frac{1}{M_*^2}\partial_\mu(\mathcal{X})J_B^\mu\,, \tag{5.32}$$

with $\mathcal{X}$ being a arbitrary quantity related with the modified gravity under question. Such concept somewhat emerged early on from the first modifications to Gravitational Baryogenesis [195] and later adopt in diverse works of modified gravity in the context of GB (see [73, 74, 75, 76, 77, 78, 79, 196, 197] for examples). With this being said, for $f(R,\mathcal{T}^2)$ gravity the following terms will be considered

$$\frac{1}{M_*^2}\int d^4x\sqrt{-g}\,\partial_\mu(\mathcal{T}^2)J_B^\mu\,, \tag{5.33}$$

$$\frac{1}{M_*^2}\int d^4x\sqrt{-g}\,\partial_\mu(f(R,\mathcal{T}^2))J_B^\mu\,, \tag{5.34}$$

that consequently lead to the asymmetries

$$\frac{n_b}{s} \simeq -\frac{15g_b}{4\pi^2 g_*}\frac{\dot{\mathcal{T}}^2}{M_*^2 T}\bigg|_{T_D}\,. \tag{5.35}$$

$$\frac{n_b}{s} \simeq -\frac{15g_b}{4\pi^2 g_*}\frac{\dot{R}f_{,R}+\dot{\mathcal{T}}^2 f_{,\mathcal{T}^2}}{M_*^2 T}\bigg|_{T_D}\,, \tag{5.36}$$

respectively.

Before starting to employ the cosmological description of $f(R,\mathcal{T}^2)$ to obtain the previous asymmetries, it is fundamental to do a careful consideration about the parameters M_* and T_D, as these play a pivotal role and demand precise consideration. In the original framework of gravitational baryogenesis, as outlined in [72], it is not necessary for M_* to reach the Planck scale. For instance, in cases where baryon number violation (B-violation) is governed by the Majorana mass M_R of the right-handed neutrino—a scenario involving soft B-violation—the expression in Eq. (3.26) avoids violating unitarity up to the Planck mass, even with $M_*^2 = M_R M_{Pl}$ [72]. Consequently, the cutoff scale for the $\partial_\mu R$ coupling can be lowered as needed to facilitate baryogenesis. For the additional couplings introduced in an ad hoc fashion, the cutoff scale will vary based on specific models and numerical results that lead to a successful baryogenesis scenario. Once such a scenario is identified it can be compared to the LHC energy scale offering a way to exclude these terms if M_* falls below the detection threshold of the LHC, as these interactions would have been detected up to this scale.

For the decoupling temperature, T_D, it is generally recognized in the literature that during the radiation-dominated era following inflation, the decoupling temperature T_D is approximately equivalent to the inflationary scale M_I, where $M_I \simeq 1.6\times 10^{16}$ GeV, based on the upper limit imposed by constraints on tensor mode fluctuations [198]. Although this approximation is widely accepted, we will re-examine this assumption in a more critical light. During the slow-roll phase of inflation, as inflation comes to an end, the scalar field oscillates around the potential minimum, thereby initiating the reheating phase—a crucial process for the thermalization of the Universe. Consequently, if baryogenesis is assumed to occur during the radiation-dominated era following inflation, the decoupling temperature must satisfy the condition $T_D < T_{RD} < M_I$, where T_{RD} denotes the temperature at which the Universe transitions to radiation domination, or equivalently, the reheating temperature. The exact value of T_{RD} is contingent on the inflationary model employed (see detailed discussions in [199, 200, 201, 202]). While in principle T_{RD} can approach the Grand Unified Theory (GUT) scale, around $\sim 10^{16}$ GeV, such high values are often considered unrealistic. Therefore, the assumption $T_D \approx M_I$ is problematic, as it would imply that T_{RD} is nearly equal to M_I, a scenario rarely achieved in typical inflationary models. To maintain generality, we refrain from adopting a specific inflationary model. Instead, we take M_I as an upper bound, consistent with the small temperature fluctuations observed in the CMB. In this context, we adopt the conservative range $T_{RD} \lesssim 10^9 - 10^{14}$ GeV [96, 198, 202, 203, 204]. This broader range, coupled with the condition $T_D \approx T_{RD}$, allows for more flexibility in the possible values of T_D, compared to the restrictive assumption $T_D \simeq M_I$.

Establishing a lower bound for T_D is more challenging. Within the temperature range of 100 GeV to 10^{12} GeV, gauge interactions and sphaleron processes maintain thermal equilibrium [112]. Furthermore, the lower limit of T_D is closely tied to the specific mechanism responsible for baryon number violation, which is essential for gravitational baryogenesis. An examination of this issue will be presented later in this section.

5.3.1 Couplings between $\partial_\mu(R)$ and J^μ

(i) Model $n = 1/4$:

The model with $n = 1/4$ as interesting cosmological equations with the modified Friedmann equation being equal to the standard Friedmann equation in GR

$$H^2 = \frac{\rho}{3M_{Pl}^2}\,, \tag{5.37}$$

and the modified acceleration equation being give by

$$\dot{H} + 2H^2 = -\frac{\eta}{192^{1/4}}\rho^{1/2}\,. \tag{5.38}$$

Another interesting aspect of this model is the fact that the coupling constant in this scenario is dimensionless and κ couples to this parameter. By contracting both equations, we derive the following differential equation

$$\dot{H} + 2H^2 + z(\eta)H = 0\,, \tag{5.39}$$

with

$$z(\eta) = \frac{\eta\sqrt{3}M_{Pl}}{192^{1/4}}\,, \tag{5.40}$$

and that yields the solution

$$H(t) = \frac{z}{e^{zt} - 2}\,. \tag{5.41}$$

Having an expression for the Hubble parameter allows to compute R and $\dot{R}$. For a flat FLRW metric with signature $(-,+,+,+)$ the Ricci scalar is given by

$$R = 6(\dot{H} + 2H^2)\,, \tag{5.42}$$

and taking the time derivative provides

$$\dot{R} = 6(\ddot{H} + 4H\dot{H}) . \tag{5.43}$$

Using Eq. (5.38) the Ricci scalar has the form

$$R = -6\left(\frac{\eta}{192^{1/4}}\rho^{1/2}\right) , \tag{5.44}$$

and substituting Eq.(5.41) into Eq.(5.37) we obtain the time dependent expression for the energy density

$$\rho(t) = 3M_{Pl}^2\left(\frac{z}{e^{zt}-2}\right)^2 , \tag{5.45}$$

allowing to write the Ricci scalar as

$$R = -6\left(\frac{\eta\sqrt{3}M_{Pl}}{192^{1/4}}\frac{z}{e^{zt}-2}\right) , \tag{5.46}$$

and its time derivative as

$$\dot{R} = 6\left[\frac{\eta\sqrt{3}M_{Pl}e^{zt}}{192^{1/4}}\left(\frac{z}{e^{zt}-2}\right)^2\right] . \tag{5.47}$$

We can relate the time of decoupling with the temperature of decoupling by using the equation that relates the total radiation density with the energy of all relativistic species (Eq.(2.52)) [96]

$$\rho(t) = \frac{\pi^2}{30}g_* T^4 , \tag{5.48}$$

and solving for t_D. Substituting this result into Eq. (5.45) gives the relation

$$\left(\frac{z}{e^{zt_D}-2}\right)^2 = \frac{\pi^2 g_*}{90M_{Pl}^2}T_D^4 , \tag{5.49}$$

and

$$e^{zt_D} = \frac{3z\sqrt{10}M_{Pl}}{\pi g_*^{1/2}T_D^2} + 2 , \tag{5.50}$$

so that Eq. (5.47) can be rewritten as

$$\dot{R} = \left(\frac{\sqrt{15}(\frac{9}{2})\pi g_*^{1/2}\eta^2 M_{Pl}^2 T_D^2 + 2(3^{5/4})\pi^2\eta g_* T_D^4}{90\sqrt{2}M_{Pl}}\right) . \tag{5.51}$$

Finally, from this result, the asymmetry relation (3.28) is then given by

$$\frac{n_b}{s} \simeq -\frac{15g_b}{4\pi^2 g_* 90\sqrt{2}M_*^2 M_{Pl}}\left[\left(\frac{9}{2}\right)\pi\sqrt{15}g_*^{1/2}\eta^2 M_{Pl}^2 T_D + 2(3^{5/4})\pi^2\eta g_* T_D^3\right] . \tag{5.52}$$

By setting $g_b \sim \mathcal{O}(1)$ and $g_* = 106$ (these two parameters will remain fixed throughout this work), along with $M_* = M_{Pl}$ and the specified range for T_D, the asymmetry consistently displays negative values, regardless of the parameter η or the value of M_*. This negative asymmetry suggests a preference for the production of antimatter over matter, thereby making this scenario untenable.

(ii) Model $n=1/2$:

For the case with $n=1/2$ the modified cosmological equations read

$$H^2=\left(\frac{\kappa}{3}+\frac{\eta'\sqrt{3}}{9}\right)\rho\ ,\ \dot{H}+H^2=-\left(\frac{\kappa}{3}+\frac{\eta' 2\sqrt{3}}{9}\right)\rho \tag{5.53}$$

and by using the full expression for η' can be recast as

$$H^2=\left(\frac{3+\eta\sqrt{3}}{9}\right)\frac{\rho}{M_{Pl}^2}, \tag{5.54}$$

$$\dot{H}+H^2=-\left(\frac{3+\eta 2\sqrt{3}}{9}\right)\frac{\rho}{M_{Pl}^2}, \tag{5.55}$$

respectively.

By substituting Eq. (5.54) into Eq. (5.55) yields the differential equation

$$\dot{H}+\left(\frac{3\eta+2\sqrt{3}}{\eta+\sqrt{3}}\right)H^2=0, \tag{5.56}$$

that has the analytical solution

$$H(t)=\alpha(\eta)t^{-1}, \tag{5.57}$$

with

$$\alpha(\eta)=\frac{\eta+\sqrt{3}}{3\eta+2\sqrt{3}}, \tag{5.58}$$

corresponding to a power law for the scalar factor, $a(t)\sim t^{\alpha}$. Utilizing the solution derived for H, Eq. (5.43) can be reformulated as

$$\dot{R}=-12\alpha(\eta)\left(\frac{2\alpha(\eta)-1}{t^3}\right). \tag{5.59}$$

The solution for the Hubble parameter allows to derive a time-dependent expression for ρ. By substituting this solution into the continuity equation (4.47), we obtain

$$\dot{\rho}(t)+2t^{-1}\rho(t)=0, \tag{5.60}$$

that has the solution

$$\rho(t)=\rho_0 t^{-2}, \tag{5.61}$$

where ρ_0 is a constant. By plotting this solution in conjunction with the solution for H into Eq. (5.54) we find

$$\rho_0=\frac{3\sqrt{3}\eta+9}{(3\eta+2\sqrt{3})^2}M_{Pl}^2, \tag{5.62}$$

that allows to rewrite (5.48) as

$$t_D=\left(\frac{30\rho_0}{\pi^2 g_*}\right)^{1/2}T_D^{-2}. \tag{5.63}$$

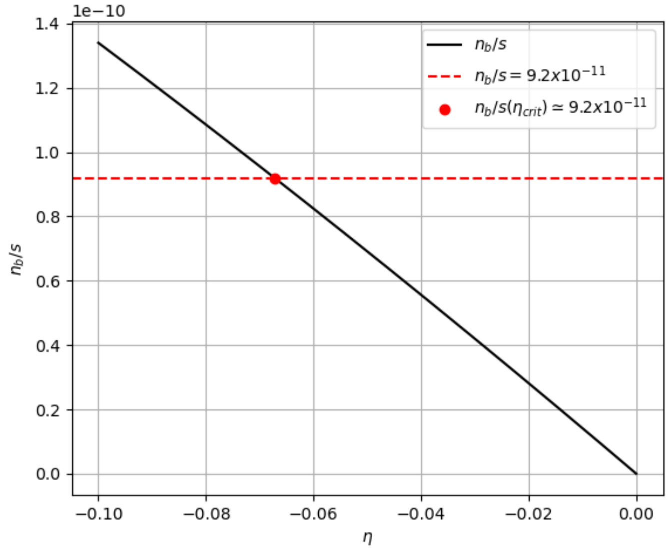

Figure 5.1: Plot of $\frac{n_b}{s}$ vs η. The black line shows the evolution of $\frac{n_b}{s}(\eta)$, for the $n = 1/2$ model, the dashed red line indicates the observation constraint for $\frac{n_b}{s}$ and the red dot marks the point where $\frac{n_b}{s}(\eta_{crit}) = 9.1998 \times 10^{-11}$ with $\eta_{crit} \approx -0.06726$ being the last rounded numerical value before the observable constraint is not satisfied.

Combining Eqs. (5.59) and (5.63) into Eq.(3.28) results in

$$\frac{n_b}{s} \simeq \frac{45\pi\alpha(\eta)\,(2\alpha(\eta)-1)\,g_s^{1/2} g_b}{M_*^2 (30\rho_0)^{3/2}} T_D^5 \,. \tag{5.64}$$

For $\eta > 0$, the asymmetry produced by the previous equation is consistently negative, implying the generation of antimatter rather than matter, making this scenario unsuitable for successful baryogenesis. However, by considering $\eta < 0$, the model can generate an acceptable asymmetry. Furthermore, when exploring decoupling temperatures below 10^{12} GeV and M_* values below the LHC energy scale, successful baryogenesis scenarios with viable values for η were identified. Specifically, with $T_D = 10^{11}$ GeV and $M_* = 9 \times 10^3$ GeV, the critical value of η was found to be $\eta_{crit} = -0.00513$. Consequently, cases within this framework are deemed nonviable due to the lack of any observed B-violating interactions at these energy scales. For $T_D = 1 \times 10^{14}$ GeV and $M_* = 1 \times 10^{12}$ GeV, the plot of $\frac{n_b}{s}(\eta)$ in Fig. 5.1 demonstrates that successful baryogenesis can be achieved with a small absolute value of the coupling constant η. This suggests that the additional term $\mathcal{T}^2$ can significantly influence the system without requiring a large constant. The effect of $\mathcal{T}^2$ primarily stems from additional terms such as $\frac{\eta'\sqrt{3}}{9}$ and $2\frac{\eta'\sqrt{3}}{9}$ in the cosmological equations, introducing new dynamics into the cosmological description. Additionally, using Eqs. (5.54) and (5.55), $\dot{R}$ can be expressed as

$$\dot{R} = -\frac{2\eta\sqrt{3}}{3}\frac{\dot{\rho}}{M_{Pl}^2}\,, \tag{5.65}$$

where $\dot{\rho}$ can be derived from Eq. (5.61). The results in Fig. 5.1 show that the magnitude of η required for successful baryogenesis mirrors the behavior seen in the GR case, where

$$\dot{R} = (1-3w)\frac{\dot{\rho}}{3M_{Pl}^2}\,, \tag{5.66}$$

at very high energy scales, and typical gauge fields and matter contents exhibit a trace anomaly characterized by an equation of state (EOS) with $(1 - 3w \sim 10^{-2} - 10^{-1})$ [72, 205]. This allows Eq. (5.66) to be used to calculate the asymmetry. In other words, the results for η correspond to $1-3w \sim 10^{-2}-10^{-1}$, indicating similar behavior between this scenario and GR, suggesting a significant resemblance in the underlying physical mechanisms described by both frameworks.

Another crucial point is that η_{crit} is larger than the constraint on η derived from BBN, as outlined in [188]. This means that the constraint imposed by gravitational baryogenesis does not align with the fundamental BBN constraint, preventing this specific case from satisfying both successful baryogenesis and BBN requirements. However, given that the value of η derived from the baryogenesis constraint is relatively small, it is possible to develop a model similar to the one discussed, which addresses the baryon asymmetry problem while minimizing the impact of the $\mathcal{T}^2$ scalar. This would ensure consistency with BBN. Specifically, such a model could involve a dynamic coupling constant η that decreases after the baryogenesis epoch, eventually converging towards GR or $f(R)$ gravity.

The case with η constrained, (4.53), leads to a new framework as the cosmological equations are different from the previous ones with $w=1/3$. With w not being specified, the cosmological equations read

$$H^2 = \beta(\eta_*,w)\frac{\rho}{3M_{Pl}^2}\,, \tag{5.67}$$

$$\dot{H}+H^2 = -\delta(\eta_*,w)\frac{\rho}{3M_{Pl}^2}\,, \tag{5.68}$$

with η_* representing η obtained from Eq. (4.53) and $\beta(\eta_*,w)$, $\delta(\eta_*,w)$ being given by

$$\beta(\eta_*,w) \equiv 1+\eta_* C_{Frd}(\frac{1}{2},w)\ ,\ \delta(\eta_*,w) \equiv \frac{1+3w+2\eta_* C_{Acc}(\frac{1}{2},w)}{2}\,. \tag{5.69}$$

Substituting once again Eq. (5.67) into Eq. (5.68) gives the differential equation

$$\dot{H}+\frac{\beta(\eta_*,w)+\delta(\eta_*,w)}{\beta(\eta_*,w)}H^2 = 0\,, \tag{5.70}$$

that has the solution

$$H = \lambda t^{-1}\,, \tag{5.71}$$

where λ is

$$\lambda(\eta_*,w) \equiv \frac{\beta(\eta_*,w)}{\beta(\eta_*,w)+\delta(\eta_*,w)}\,. \tag{5.72}$$

The time derivative of the Ricci scalar is then given by

$$\dot{R} = -12\lambda\left(\frac{2\lambda-1}{t^3}\right)\,. \tag{5.73}$$

The important difference of this special case resides in the form of the continuity equation that is now is given by

$$\dot{\rho} = -4H\rho\,, \tag{5.74}$$

that has the solution

$$\rho = \rho_c t^{-4\lambda}\,, \tag{5.75}$$

with ρ_c being a positive constant with units $\mathrm{GeV}^{4+4\lambda}$.

Tabela 5.1: Successful cases for different w for the coupling between $\partial_\mu R$ and J^μ. The values for η_* and n_B/s are rounded.

w	T_D [GeV]	M_* [GeV]	ρ_c [GeV$^{4+4\lambda}$]	η_*	$\frac{n_B}{s}/10^{-11}$
0.3	1.95×10^{10}	M_{Pl}	1×10^{45}	0.010825	8.915146
$-1/3$	1.75×10^{10}	M_{Pl}	1×10^{45}	2.508041	8.716503
$-2/3$	2×10^{7}	1×10^{5}	2×10^{-6}	-0.986178	8.979037
-0.7	2×10^{7}	3×10^{4}	1×10^{9}	-0.919929	8.944976

Using once again Eq.(5.48) the decoupling time-temperature relation is

$$t_D = \left(\frac{\pi^2 g_*}{30}\right)^{-1/4\lambda} T_D^{-1/\lambda}\rho_c^{1/4\lambda}\,, \tag{5.76}$$

allowing to write Eq. (3.28) as

$$\frac{n_B}{s} \simeq \frac{45 g_b (\pi^2 g_*)^{\frac{3}{4\lambda}-1}\lambda(2\lambda-1)}{30^{\frac{3}{4\lambda}} M_*^2 \rho_c^{\frac{3}{4\lambda}}} T_D^{\frac{3}{\lambda}-1}\,. \tag{5.77}$$

As previously noted, the case of $w = 1/3$ leads to $\eta_* = 0$, resulting in no asymmetry generation, as $\eta_* = 0$ gives $\lambda = 0.5$, which in turn leads to $\dot{R} = 0$. However, one can consider cases where $w \approx 1/3$, as discussed earlier, using the approximation $(1-3w \sim 10^{-2}-10^{-1})$. Before assigning specific values to w, it is crucial to examine how the asymmetry expression behaves in relation to λ. The key finding here is that the evolution of $\lambda(w)$ decreases inversely with w. Additionally, when $0 < \lambda < \frac{1}{2}$, which corresponds to $w > \frac{1}{3}$, a negative asymmetry arises, rendering this scenario non-viable and excluding any non-thermal components with $w > \frac{1}{3}$, such as stiff matter ($w = 1$).

A particularly notable effect occurs when $\lambda < 0$, where the decoupling temperature, which typically enhances asymmetry, behaves inversely. This inversion happens because when $\frac{3}{\lambda} - 1 < 0$, the decoupling temperature appears in the denominator of the asymmetry expression. At the same time, the constant ρ_c acts to amplify the asymmetry, as it moves into the numerator when $\frac{3}{4\lambda} < 0$. Similarly, the inverse behavior of T_D is observed when $\lambda > 3$, though in this case, ρ_c does not fully counterbalance the effect.

The cases that successfully generate an acceptable asymmetry are summarized in Table 5.1. The first case pertains to radiation, using $1-3w \sim 10^{-2}-10^{-1}$, as mentioned earlier. The second case involves an effective perfect fluid representing negative curvature, while the third and fourth cases are associated with a form of dark energy. These successful scenarios, combined with the fact that this model naturally aligns with the standard energy density evolution in a radiation-dominated era, underscore the model's relevance. Moreover, the conclusion that the influence of $\mathcal{T}^2$ in this model leads to an effective coupling constant, composed of the General Relativity (GR) coupling constant and an additional term proportional to η',further highlights how subtle modifications to the GR framework could potentially address the long-standing issue of baryonic asymmetry. This model's ability to integrate minor adjustments into GR offers a promising approach for resolving the persistent challenge of baryonic asymmetry.

(iii) Model $n = 1$:

The $n = 1$ case has the following modified Friedmann equations

$$H^2 = \frac{\kappa}{3}\rho + \frac{2}{3}\eta'\rho^2\,, \tag{5.78}$$

$$\dot{H}+H^2=-\frac{\kappa}{3}\rho-\frac{2}{3}\eta'\rho^2\,, \tag{5.79}$$

respectively.

Once again, substituting (5.78) into (5.79) leads to the differential equation

$$\dot{H}+2H^2=0\,, \tag{5.80}$$

that yields the solution

$$H(t)=\frac{1}{2}t^{-1} \tag{5.81}$$

leading to $a\propto t^{1/2}$. Using Eqs. (5.43) and (5.81) leads to $\dot{R}=0$ (and $R=0$ also), allowing to conclude that there is no asymmetry generated by Eq.(3.26) in this case. Although the Friedmann equations for this case deviate strongly from GR due to the presence of the quadratic term, ρ^2, from the baryogenesis point of view, this case behaves exactly as the case of $w=1/3$ in GR.

5.3.2 Couplings between $\partial_\mu\left(\mathcal{T}^2\right)$ and J^μ

(i) Model $n=1/4$:

Using the right side of Eq.(4.35) for this case one has

$$\mathcal{T}^2=12M_{Pl}^4\left(\frac{z}{e^{zt}-2}\right)^4\,, \tag{5.82}$$

and taking into account Eqs. (5.49) and (5.50) provides the following expression for $\dot{\mathcal{T}}^2$

$$\dot{\mathcal{T}}^2=-48\pi^4 g_*^2 T_D^8\left[\frac{3(\frac{3}{64})^{1/4}\eta\sqrt{10}M_{Pl}^2+2\pi g_*^{1/2}T_D^2}{90^{5/2}M_{Pl}}\right]\,, \tag{5.83}$$

resulting in the asymmetry

$$\frac{n_b}{s}\simeq\frac{g_b g_*\pi^3 T_D^7}{130\sqrt{10}M_*^2 M_{Pl}}\left[3\left(\frac{3}{64}\right)^{1/4}\eta\sqrt{10}M_{Pl}^2+2\pi g_*^{1/2}T_D^2\right]\,. \tag{5.84}$$

The expression for this scenario fails to generate an acceptable asymmetry, as it consistently suppresses the observable value for asymmetry. The contribution from $\mathcal{T}^2$ excessively enhances the asymmetry. Thus, this case is not viable for achieving successful baryogenesis.

(ii) Model $n=1/2$:

Using the results for $n=1/2$ from subsection 5.3.1 and Eq. (4.35) we can write

$$\mathcal{T}^2=\frac{4}{3}\rho^2=\frac{4}{3}\rho_0^2 t^{-4}\,, \tag{5.85}$$

leading to

$$\dot{\mathcal{T}}^2=-\frac{16}{3}\rho_0^2 t^{-5}\,, \tag{5.86}$$

where ρ_0 is given by Eq. (5.62). This results leads to the asymmetry

$$\frac{n_b}{s}\simeq\frac{20\pi^3 g_*^{3/2}g_b}{(30)^{5/2}M_*^2(\rho_0)^{1/2}}T_D^9\,. \tag{5.87}$$

Tabela 5.2: Successful cases for different w for the coupling between $\partial_\mu \mathcal{T}^2$ and J^μ. The values for η_* and n_B/s are rounded.

w	ρ_c [GeV$^{4+4\gamma}$]	η_*	$\frac{n_B}{s}/10^{-11}$
1	3×10^{56}	$-1/8$	9.132028
0.3	1×10^{45}	0.010825	9.056777
$-1/3$	1×10^{45}	2.508041	9.146172

In this scenario no acceptable asymmetry is produced, as it consistently exceeds the imposed constraints. The primary factor influencing this behavior is the exponent of the decoupling temperature. Yet again, the contribution from the new scalar significantly amplifies the asymmetry, but to an excessive degree.

Considering the constrained case (4.53) and Eq.(5.75) the scalar $\mathcal{T}^2$ is now given by

$$\mathcal{T}^2(w) = (1+3w^2)\rho_c^2 t^{-8\lambda}\,, \tag{5.88}$$

leading to

$$\dot{\mathcal{T}}^2(w) = -8\lambda(1+3w^2)\rho_c^2 t^{-8\lambda-1}\,. \tag{5.89}$$

Using Eq.(5.76), the asymmetry is then given by

$$\frac{n_b}{s} \simeq \frac{g_b\lambda(1+3w^2)(\pi^2 g_*)^{1+1/4\lambda}}{(30)^{1+1/4\lambda}\rho_c^{1/4\lambda}M_*^2} T_D^{7+\frac{1}{\lambda}}\,. \tag{5.90}$$

In analyzing the previous equation, unlike the case of the $\partial_\mu R$ coupling, no value of w results in a negative asymmetry, as the expression $1+3w^2$ remains positive for all real values of w. Additionally, the decoupling temperature parameter once again proves to be critical in determining the viability of this scenario, as it controls whether the resulting asymmetry aligns with observational constraints. As previously noted, λ decreases as w increases. Therefore, to fully explore the range of possible values for w, one can fix $M_* = M_{Pl}$ and set $T_D = 1\times10^7$ GeV, which helps mitigate the excessive contributions from the temperature. With this configuration, the successful cases (those where ρ_c does not become excessively large) for various values of w are summarized in Table 5.2. Two of these cases were already discussed in the previous section, while the new case, $w=1$, corresponds to a stiff fluid. Notably, the $\partial_\mu \mathcal{T}^2$ coupling can generate a substantial asymmetry for $w > \frac{1}{3}$, particularly for $w=1$. This contrasts with the behavior of the $\partial_\mu R$ coupling, which only produced successful results for $w < \frac{1}{3}$.

Moreover, the lack of successful baryogenesis when the constraint needed to reproduce the typical energy density behavior of the radiation era is not applied highlights the subtle nature of modifying the gravitational framework in the context of gravitational baryogenesis. This suggests that the contribution of the new coupling being studied is more effective when working within the standard GR framework with only minor adjustments. Once again, this finding demonstrates how even slight modifications to GR can effectively tackle the problem of asymmetry.

(iii) Model $n=1$:

For the $n=1$ case, one an use the trace of the field equations (4.40) resulting in

$$\mathcal{T}^2 = \frac{1}{2}\theta\,, \tag{5.91}$$

due to the vanishing of both the Ricci scalar and the trace of the energy-momentum tensor (the trace of

$T_{\mu\nu}$ is equal to zero for $w = 1/3$, which is related to radiation). Computing the trace of $\theta_{\mu\nu}$ by using Eq. (4.36) leads to

$$\mathcal{T}^2 = \frac{4}{3}\rho^2 , \tag{5.92}$$

which is the same result if Eq. (4.35) was used. The time derivative of $\mathcal{T}^2$ is then

$$\dot{\mathcal{T}}^2 = \frac{8}{3}\dot{\rho}\rho . \tag{5.93}$$

Considering the leading orders of ρ one has

$$\rho(t) \simeq \sqrt{\frac{3}{8\eta'}}t^{-1} , \tag{5.94}$$

that provides

$$\dot{\mathcal{T}}^2 = -\eta'^{-1}t^{-3} , \tag{5.95}$$

and the decoupling time

$$t_D = \sqrt{\frac{3}{8\eta'}}30\pi^{-2}g_*^{-1}T_D^{-4} . \tag{5.96}$$

Combining all the results the asymmetry is given by

$$\frac{n_b}{s} \simeq \frac{(8/3)^{3/2}g_b g_*^2\pi^4\eta^{1/2}}{7200M_{Pl}^3M_*^2}T_D^{11} . \tag{5.97}$$

Upon evaluating the previous expression, the term T_D^{11} requires a significantly high value for M_* to counterbalance the temperature component and achieve an observationally consistent baryon asymmetry. Setting $M_* = M_{Pl}$ and adjusting η' for varying decoupling temperatures (T_D), we identify a relationship between the decoupling temperature and the corresponding magnitude of η. For instance, at a decoupling temperature of 1×10^{11} GeV, η reaches the order of 10^{-84}, with a critical value of $\eta_{crit} = 1.2246\times10^{-84}$, which, though unphysical, produces an acceptable asymmetry: $\frac{n_b}{s} \simeq 9.1996\times10^{-11}$. However, for a lower decoupling temperature of 1×10^{8} GeV, a comparable asymmetry is achieved with $\eta = 1.224664\times10^{-18}$, a value that, although lower, remains extremely small and renders the scenario unlikely. These findings demonstrate an inverse relationship between the decoupling temperature and the magnitude of η required to sustain a viable asymmetry. For $T_D = 2\times10^{7}$ GeV, values of η at or below 2.919×10^{-3} are sufficient to produce the observed asymmetry. The behavior of $\frac{n_b}{s}(\eta)$ for this case is illustrated in Fig. 5.2. However, a significant complication arises when η takes on positive values, particularly in the context of late-time cosmology. As pointed out by Roshan et al. [189], models where $\eta > 0$—bearing in mind that the sign in this study is reversed—fail to yield a stable, late-time accelerated phase. This limitation implies that the model cannot simultaneously account for both the matter-antimatter asymmetry and the universe's late-time accelerated expansion. At the lower bound of $T_D = 10^7$ GeV, the necessary η values rise to the order of 10^4. Thus, if the goal is to generate asymmetry at temperatures around 10^7 GeV, the resulting large η values would cause the additional term in the modified Friedmann equations to dominate the cosmological evolution.

Moreover, the requirement for $T_D < 10^9$ GeV to achieve asymmetry with a physically reasonable value of η is particularly interesting. This constraint also appears in supergravity theories to prevent excessive gravitino production. In traditional supergravity models, a similar upper bound on the reheating temperature is enforced to avoid late-time gravitino decays, which could disrupt Big Bang Nucleosynthe-

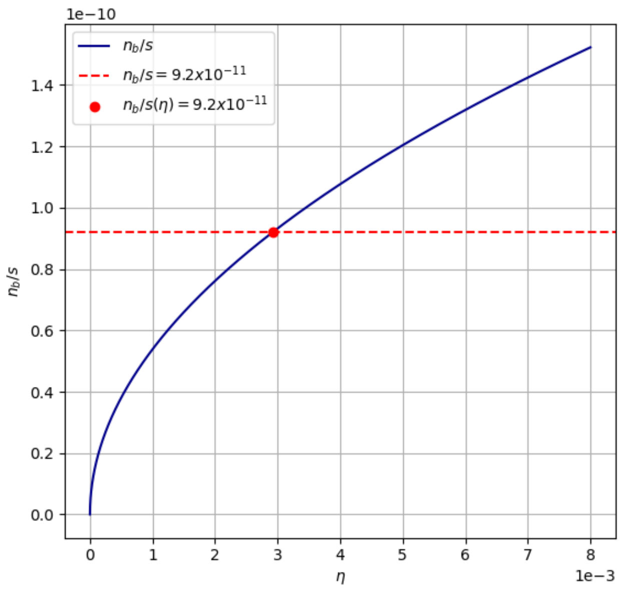

Figure 5.2: Plot of $\frac{n_b}{s}$ vs η for the asymmetry generated from coupling term (5.33). The dark blue line shows the evolution of $\frac{n_b}{s}(\eta)$, the dashed red line indicates the observation constraint for the asymmetry and the red dot marks the point where $\frac{n_b}{s}(\eta_{crit}) \approx 9.18443 \times 10^{-11}$ with $\eta_{crit} = 2.919 \times 10^{-3}$.

sis (BBN) [206]. This parallel underscores the commonality between the decoupling temperature constraints in this model and those found in supergravity frameworks. Furthermore, supergravity models also feature prominently in inflationary scenarios, with some predicting reheating temperatures consistent with the values considered in this analysis [207].

5.3.3 Couplings between $\partial_\mu \left(f(R,\mathcal{T}^2)\right)$ and J^μ

(i) Model $n = 1/4$:

Combining the results from Sections 5.3.1 and 5.3.2, the expression from the $\partial_\mu f(R,T)$ for the $n = 1/4$ model is given by

$$\frac{n_b}{s} \simeq -\frac{g_b \pi \eta T_D}{2(192)^{1/4} g_*^{1/2} M_{Pl} M_*^2} \left[(\sqrt{3} - 2(192)^{1/4}) \left(3\eta\sqrt{10}(\frac{3}{64})^{1/4} M_{Pl}^2 + 2\pi g_*^{1/2} T_D^2 \right) \right]. \tag{5.98}$$

As seen in the case where $n = 1$ for the $\partial_\mu \mathcal{T}^2$ coupling, setting $M_* = M_{Pl}$ and performing computational calculations revealed an inverse relationship between the decoupling temperature T_D and the parameter η. Specifically, as T_D increases, the value of η required to meet observational constraints on baryonic asymmetry decreases. This outcome is due to the interaction between the Ricci scalar and the scalar term $\mathcal{T}^2$, which enables the generation of an acceptable asymmetry. This behavior contrasts with previous cases involving the $\partial_\mu R$ and $\partial_\mu \mathcal{T}^2$ couplings. For example, with $T_D = 10^8$ GeV and $M_* = M_{Pl}$, the plot of the baryon-to-entropy ratio $\frac{n_b}{s}(\eta)$ in Figure 5.3 shows a rapid increase in asymmetry with rising η, highlighting the strong dependence on the coupling parameter.

(ii) Model $n = 1/2$:

For $n = 1/2$, using the results from Sections 5.3.1 and 5.3.2 the asymmetry is given by

$$\frac{n_b}{s} \simeq \frac{15 g_b g_*^{1/2} \pi T_D^5}{M_*^2} \left[\frac{3\alpha(\eta)(2\alpha(\eta) - 1)}{(30\rho_0)^{3/2}} - \frac{\eta}{10^{1/2}(\rho_0)^{1/2} 30 M_{Pl}^2} \right]. \tag{5.99}$$

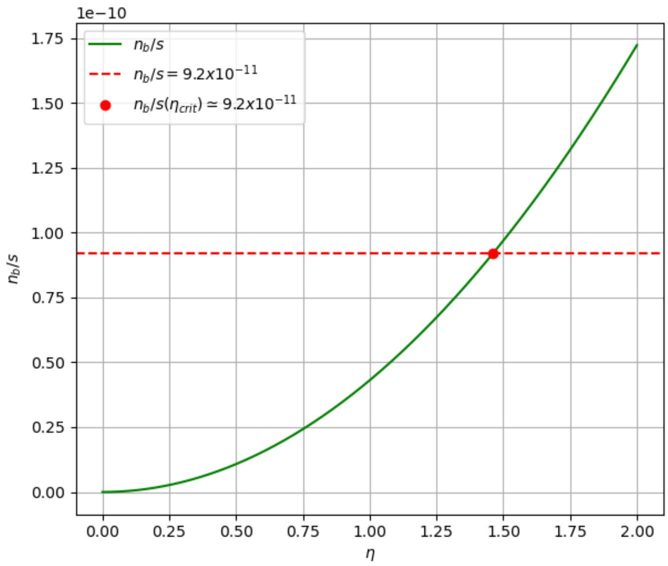

Figure 5.3: Plot of $\frac{n_b}{s}$ vs η for the asymmetry generated from the general coupling for the $n=1/4$ model. The green line shows the evolution of $\frac{n_b}{s}(\eta)$, the dashed red line indicates the observation constraint for the asymmetry and the red dot marks the point where $\frac{n_b}{s}(\eta_{crit}) \approx 9.1988327\times10^{-11}$ with $\eta_{crit} = 1.4615892317846357$.

This result illustrates the interaction between two sources of asymmetry: the Ricci scalar, represented by the first term in the parentheses, and the scalar $\mathcal{T}^2$, represented by the second term. The decoupling temperature plays a crucial role in this interaction. As discussed in Section 5.3.1, the term associated with R becomes negative when η is positive. Similarly, the contribution from $\mathcal{T}^2$ also remains negative for $\eta > 0$. Therefore, selecting positive values of η results in a negative overall asymmetry, which signifies an imbalance in favor of anti-matter. In the $n=1/2$ model for the $\partial_\mu R$ coupling, specific conditions produce asymmetries consistent with observational data, particularly when the parameter M_* is below the energy scale accessible at the LHC, and for realistic values of η. These results are valid for decoupling temperatures below 10^{12} GeV. For instance, at a decoupling temperature of $T_D = 10^{11}$ GeV and with $M_* = 9\times10^3$ GeV, the critical value of η was found to be $\eta_{crit} = -0.000852$. However, such scenarios have been considered unrealistic. For a decoupling temperature of $T_D = 1\times10^{14}$ GeV and $M_* = 1\times10^{12}$ GeV, the evolution of the baryon-to-entropy ratio, $\frac{n_b}{s}(\eta)$, is depicted in Figure 5.4. As before, successful baryogenesis is achieved with higher values of η, driven by the interplay between the Ricci scalar and the scalar $\mathcal{T}^2$. If the contribution were solely from the term associated with R, the result would align with what was previously obtained in Section 5.3.1. However, the inclusion of the scalar $\mathcal{T}^2$ significantly raises the value of η, underscoring its essential role in the baryogenesis mechanism.

Supporting this conclusion, the findings from Section 5.3.2 indicate that the coupling of $\partial_\mu\mathcal{T}^2$ alone leads to an excessive increase in baryonic asymmetry. In the more general scenario of $f(R,\mathcal{T}^2)$, however, the Ricci scalar and the additional terms derived from $f_{\mathcal{T}^2}$ work together to moderate the excessive contribution of the scalar $\mathcal{T}^2$.

Regarding the case with the constraint, the expression for the generated asymmetry is

$$\frac{n_b}{s} \simeq \frac{15 g_b \gamma}{\pi^2 g_* M_*^2}\left[\frac{3(2\gamma-1)(\frac{\pi^2 g_*}{30})^{3/4\gamma} T_D^{3/\gamma-1}}{p_c^{3/4\gamma}} + \frac{\eta_*(1+3w^2)^{1/2}(\frac{\pi^2 g_*}{30})^{1+1/4\gamma} T_D^{3+1/\gamma}}{p_c^{1/4\gamma} M_{Pl}^2}\right]. \tag{5.100}$$

One can see that exists again an interplay between both contributions from the different scalars. Some subspaces of the model parameter space result in a asymmetry that is negative rendering these cases non-viable. Considering $T_D = 1\times10^{13}$ GeV and $M_* = 1\times10^{12}$ GeV two successful cases

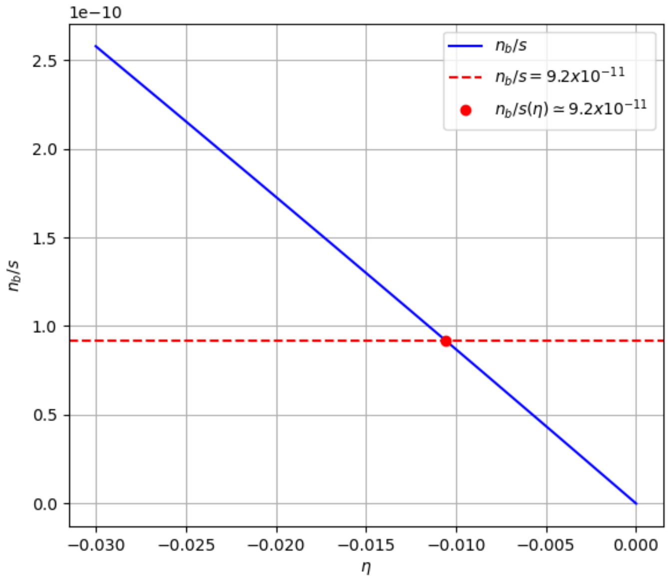

Figure 5.4: Graphical representation of $\frac{n_b}{s}$ vs η derived from the general coupling term $f(R,\mathcal{T}^2)$ for the case $n = 1/2$. The blue line represents $\frac{n_b}{s}(\eta)$, the dashed red line indicates the observation constraint for $\frac{n_b}{s}$ and the red dot marks the point where $\frac{n_b}{s}(\eta_{crit}) \approx 9.195741 \times 10^{-11}$ with $\eta_{crit} = -0.01058$.

where for, one for $w = 0.3$ with $\rho_c = 7.5 \times 10^{32}$ giving $n_B/s \simeq 9.06400 \times 10^{-11}$ and for $w = -1/3$ with $\rho_c = 8.8 \times 10^{32}$ resulting in $n_B/s \simeq 9.043081 \times 10^{-11}$. These results appear less favorable when compared to those obtained from each individual coupling separately. This outcome arises from the interplay between the different couplings, where both contributions exhibit limitations that often invalidate the resulting asymmetry. For instance, in the case of $w = 1$, the parameter η_* is negative rendering the contribution of $f_{\mathcal{T}^2}$ negative, which necessitates a compensating contribution from the sector associated with the derivative of the Ricci scalar to counterbalance this negative value. However, for $w = 1$, the contribution from the derivative of the Ricci scalar is also negative, thereby failing to provide the required compensation.

(iii) Model $n = 1$:

For $n = 1$, there is no contribution to the asymmetry from the Ricci scalar because, in this case, $R = 0$. By applying Eq.(5.93) and the decoupling time from Eq.(5.96), the asymmetry in this scenario is given by

$$\frac{n_b}{s} \simeq \frac{(8/3)^{3/2} g_b g_*^2 \pi^4 \eta^{3/2}}{7200 M_{Pl}^9 M_*^2} T_D^{11} \,. \tag{5.101}$$

This case closely resembles the scenario for $n = 1$ in the $\partial_\mu \mathcal{T}^2$ coupling with J^μ, differing only by a factor of η'^{-1}. As a result, the behavior in this case will be identical to that described for $n = 1$ in Section 5.3.2. However, for $T_D = 10^7$ GeV with $M_* = M_{Pl}$, the values of η required to produce an acceptable asymmetry are too large to be considered viable, rendering this case nonviable.

5.3.4 Models with $n < 1/4$ and $n > 1$

Besides the three models previously analyzed, it is also possible to explore the extreme cases where $n < 1/4$ and $n > 1$ within the framework of gravitational baryogenesis. These scenarios were not initially considered, as they involve coupling constants with unnatural dimensions, hence they are referred to as extreme cases. However, we will outline a potential theoretical basis for both cases to be applied in the context of gravitational baryogenesis.

Starting with the modified Friedmann equations for $w = 1/3$, we have the following expressions

$$H^2 = \frac{\rho}{3M_{Pl}^2} + \frac{\eta' \rho^{2n}}{3} C_{Frd}\left(n, \frac{1}{3}\right), \tag{5.102}$$

$$\dot{H} + H^2 = -\frac{\rho}{3M_{Pl}^2} - \frac{\eta' \rho^{2n}}{3} C_{Acc}\left(n, \frac{1}{3}\right), \tag{5.103}$$

respectively.

Considering the high-energy scale of the early universe ($\rho \to \infty$), two distinct approximations can be made depending on whether $n < 1/4$ or $n > 1$. In the case of $n < 1/4$, the ρ term is expected to dominate over the ρ^{2n} term, since the exponent associated with ρ^{2n} is less than 1. This allows the modified cosmological equations to effectively reduce to those of GR. Conversely, for $n > 1$, the quadratic term ρ^{2n} dominates, resulting in modified Friedmann equations

$$H^2 = \frac{\eta' \rho^{2n}}{3} C_{Frd}\left(n, \frac{1}{3}\right), \tag{5.104}$$

$$\dot{H} + H^2 = -\frac{\eta' \rho^{2n}}{3} C_{Acc}\left(n, \frac{1}{3}\right). \tag{5.105}$$

It is crucial to note that these results hold only under the condition of sufficiently large energy density. If this condition is not satisfied, the parameter η' invalidates both sets of equations. Another important point to highlight is the specific case of $n = 1$. Although not treated as an extreme case in this analysis due to the unique properties it exhibits, the reasoning supporting the exclusion of $n = 1$ relates to the energy density conditions involved. The range of decoupling temperatures considered in this study, which occur after inflation and during the grand unification era, do not meet the required energy density thresholds. For the case of $n = 1$, the approximation used only applies when considering epochs such as pre-inflation or inflation. Therefore, we did not include $n = 1$ as an extreme case due to its distinctive behavior under these specific cosmological conditions.

5.3.5 B-Violation in GB

To fully achieve gravitational baryogenesis, it is necessary to consider a baryon-violating (B-violating) process that can generate the required asymmetry. While multiple B-violating processes could be examined, this discussion will remain general by focusing on a B-violating interaction represented by the operator $\mathcal{O}_B$, which has a mass dimension of $4 + m$, where $m > 0$. The rate of B-violation for this interaction is given by [72]

$$\Gamma_B = \frac{T^{2m+1}}{M_B^{2m}}, \tag{5.106}$$

where M_B represents the mass scale associated with $\mathcal{O}_B$. As previously noted, B-violating processes cease when the Hubble parameter $H(T)$ equals the interaction rate $\Gamma_B(T)$, allowing the decoupling temperature to be determined by equating the expansion rate to the interaction rate.

Such an interaction could arise from an extension to the Standard Model of particle physics or as a non-renormalizable interaction in an effective field theory. Furthermore, from the perspective of gravitational baryogenesis being rooted in supergravity theories, such theories are expected to include B-violating processes. This forms a logical connection between the interaction term driving asymmetry and the process responsible for generating it. Consequently, to adopt this perspective, constraints on the reheating temperature, T_{RD}, must be considered [208]. In supersymmetric models, especially those involving warm inflation [209], additional constraints on T_{RD} arise due to gravitino production and its associated challenges. Specifically, these constraints are imposed to: (1) protect Big Bang Nucleosynthesis (BBN) from being disrupted by late gravitino decays, and (2) prevent overclosure of the universe due to an overabundance of gravitinos. Since parameters such as the gravitino mass $m_{3/2}$ and gravitino decay processes are model-dependent, we will adopt a conservative upper limit for T_{RD}, specifically $T_{RD} < 10^9$ GeV [206, 210, 211]. In the case of the $\partial_\mu R$ coupling with $n = 1/2$, where no specific form for ρ is imposed, the first two cases in Table 5.1 have temperature constraints that prevent the B-violation process from originating in supergravity. For the unconstrained case, using Eq. (5.106), Eq. (5.54), and Eq. (5.64) with $\eta = \eta_{crit}$ and a $D = 7$ operator, we find $M_B \approx 1.96 \times 10^{14}$ GeV. This value is below the typical mass scale of Grand Unified Theories (GUTs) and may be linked to a GUT Higgs boson [212]. Similarly, using $\eta = \eta_*$, the constrained cases yield $M_B(w = 0.3) \approx 1.996 \times 10^{14}$ GeV, $M_B(w = -1/3) \approx 1.932 \times 10^{14}$ GeV, $M_B(w = -2/3) \approx 1.915 \times 10^{14}$ GeV, and $M_B(w = -0.7) \approx 1.9120 \times 10^{14}$ GeV. For the $\partial_\mu \mathcal{T}^2$ coupling with $n = 1/2$, performing the same calculations for the three constrained cases gives $M_B(w = 1) \approx 7.90 \times 10^7$ GeV, $M_B(w = 0.3) \approx 7.65 \times 10^7$ GeV, and $M_B(w = -1/3) \approx 7.40 \times 10^7$ GeV. For $n = 1$, a similar calculation with $D = 7$ yields $M_B = 1.1333 \times 10^8$ GeV. In the more general coupling $\partial_\mu f(R,\mathcal{T}^2)$ with $D = 6$, the model with $n = 1/4$ gives $M_B \approx 6.92 \times 10^8$ GeV, while for $n = 1/2$, the results are $M_B \approx 2.19 \times 10^{14}$ GeV, $M_B(w = 0.3) \approx 2.42 \times 10^{13}$ GeV, and $M_B(w = -1/3) \approx 2.34 \times 10^{13}$ GeV.

Chapter 6

Summary and conclusion

In the present thesis, the connections between the primordial Universe and modified gravity were explored, more precisely, the problems, with emphasis on matter-antimatter asymmetry, and the possible solutions stemming from modified gravity. In Chapter 1, a overview of the history behind gravity was presented, the current best model for cosmology, the problems that this model has, and how one can address them from the perspective of modified gravity. It was also given a concise introduction to differential geometry, where the main tools that would be necessary for this thesis were presented. This Chapter ended with the theoretical framework to derive General Relativity from the variational principle.

Chapter 2 was dedicated to present the Standard Model of Cosmology with emphasis on the Primordial Universe. The cosmological framework was explored combined with the thermodynamic one. In the thermodynamic side it was explored the key quantities and framework that are fundamental to the study of the asymmetry between matter and anti-matter. The four core quantities, energy density, pressure density, number density and entropy, necessary to create a concise framework to explore the asymmetry, were theoretically defined and studied. The key results presented in this Chapter were the cosmological equations and their importance to the description of the Universe, as changes to them at the hands of modified gravity where a fundamental result of this thesis and the theoretical way to defined the baryonic asymmetry using a thermal description.

In the subsequent chapter, baryogenesis,a theoretical mechanism responsible for generating the matter-antimatter asymmetry, was explored in depth. The foundational framework for constructing baryogenesis mechanisms, known as the Sakharov conditions, was introduced. These conditions consist of three key requirements: the violation of baryon number (B-violation), the violation of charge (C) and charge-parity (CP) symmetries, and a process that drives the system out of equilibrium. Together, these conditions provide a phenomenological approach to achieving the desired asymmetry. While they offer an effective blueprint for developing baryogenesis mechanisms, they are not strictly indispensable.

Following the introduction of the Sakharov conditions, three distinct baryogenesis mechanisms were discussed: electroweak baryogenesis, baryogenesis within Grand Unified Theories (GUT), and gravitational baryogenesis. Although all three mechanisms have their merits, especially the first two, they also exhibit significant limitations. The first two, in particular, are well-established within the framework of particle physics, whereas gravitational baryogenesis gives gravity a more fundamental role. This contrast inspired the exploration of these limitations in the context of modified theories of gravity.

To address this, two approaches were proposed: **Path A** and **Path B**. **Path A** involves applying scalar-tensor theories to the frameworks of electroweak baryogenesis and GUT baryogenesis, while **Path B** explores the use of $f(R, \mathcal{T}^2)$ gravity in the context of gravitational baryogenesis.

Electroweak baryogenesis is particularly interesting due to the fact of being completely built only using the Standard Model of particle physics. However, from the very start problems of this mechanism were found, with the most fundamental one being the necessity to ensure that the electroweak phase transition is a strong first-order, a constraint that is related with the so called sphaleron bound. Without solving such problem, EWB can be considered inefficient. The main way to solve this problem is to expand the particle side of the theory by including more complex sectors to the SM but in the thesis the idea was to modify the expansion rate of the Universe to relax the sphaleron bound. Additionally one must also ensure efficient baryon number violation, specifically, sphalerons must be in equilibrium during the symmetric phase. This condition can also be explored with modifications to gravity. For the GUT baryogenesis the main idea was to explore how gravity can affect such a mechanism that usually has a deep relation with the expansion rate of the Universe due to the departure of equilibrium required by the Sakharov conditions. Gravitational baryogenesis presents less fundamental short comings than the other two mechanisms but still has some problems, as scenarios where the generated asymmetry is either too small or excessive, intrinsic issues such as the instabilities, that can benefit from modifications to gravity.

In Chapter 4, two modified theories of gravity, scalar-tensor theory and $f(R,\mathcal{T}^2)$, were introduced from a theoretical standpoint. For both frameworks, the corresponding field equations were derived, along with the cosmological descriptions based on the Friedmann-Lemaître-Robertson-Walker metric, incorporating a perfect fluid to describe the matter sector.

The cosmological model developed for the scalar-tensor theory follows a three-epoch framework, comprising the radiation epoch, subdivided into two phases, the first of which is dominated by the JBD scalar, the second is characterized by radiation and ultra-relativistic matter that dominate over the scalar field and the third epoch corresponds to a matter-dominated epoch. Additionally, the connection between inflation and scalar-tensor theories was explored, with two types of inflationary scenarios, extended and hyperextended inflation, being presented. For the $f(R,\mathcal{T}^2)$ theory it developed a new constraint on the parameter η of the model $f(R,\mathcal{T}^2) = R + \eta M_{\text{Pl}}^{2-8n}(\mathcal{T}^2)^n$. More precisely, to reproduce the standard description of the radiation energy density, $\rho \propto a^{-4}$, among the three possible values of n: $n = 1/4$, $n = 1/2$, and $n = 1$, the case $n = 1/2$ arises naturally from the constraint employed, establishing a relationship between η and the barotropic coefficient w. The $n = 1/2$ case presented cosmological equations very similar to the GR ones with the addition of parts that depend on η.

In Chapter 5 the results of **Path A** and **Path B** were presented, in other words, the application of STT in the context of EWB and GUTB and the application of $f(R,\mathcal{T}^2)$. Starting by the STT results, EWB saw a positive impact from the changes to the expansion rate of the Universe, where from the two epochs considered, the scalar dominated one and the radiation dominated one, the first one presented the most impactful results. The first epoch demonstrated the ability to relax the sphaleron bound for $q < 1/2$. Additionally, an efficient baryon number violation also draws positive results from the first epoch. Although the reduced results presented, one can clearly see that modifying the expansion rate of the Universe by using a STT can be a way to help the EWB mechanism surpass the current limitation that it has.

For the GUTB, a non-inflationary model was extended in the context of STT presented positive results once more. Both the number of supermassive bosons X and the baryon number are affected by the changes in the expansion rate with a positive feedback depending on q. A more in-depth analysis is necessary because the true nature of the impact of the STT is encoded in the different processes that can occur during the asymmetry production.

Finally, Gravitational baryogenesis experienced significant advances through the adoption of the modified theory of gravity under consideration. Beyond the standard CPT violation term involving the

Ricci scalar, two novel contributions were introduced: one associated with the scalar term $\mathcal{T}^2$ and another through a general coupling expressed as $f(R,\mathcal{T}^2)$. The free parameters present in these terms were carefully examined, and a parameter subspace was excluded due to the prediction of positive results that would have been observed. It was also explored a generic and simple B-violation mechanism to fully realize GB. Consequently, this framework not only offers insights into baryogenesis but also provides a potential means to constrain these modified gravity models.

Among the three models characterized by different values of n, the $n = 1/2$ model yielded the most promising results, particularly when constrained by the condition $\rho \propto a^{-4}$. In contrast, the $n = 1/4$ and $n = 1$ models only showed favorable outcomes under specific conditions: the $n = 1/4$ model for the general coupling and the $n = 1$ model for the coupling with $\partial\mathcal{T}^2$. This suggests that these modifications—where the $n = 1/4$ model affects only the acceleration equation and the $n = 1$ model introduces a quadratic energy density term in both cosmological equations—are not sufficient to resolve the matter-antimatter asymmetry through gravitational baryogenesis. Moreover, although the $n = 1$ model adds quadratic enegy density term, it reproduces the same result as GR for radiation with $w = 1/3$, which yields a vanishing asymmetry for this case. The modifications induced by the $n = 1/2$ model in the cosmological framework are characterized by a small deviation from GR, parameterized by η. While the results for successful baryogenesis did not align with the constraints for η in this model, they demonstrate that even slight deviations from GR can significantly affect the baryonic asymmetry production through gravitational baryogenesis. Additionally, it was also explored from a theoretical point of view models that where under the considerations $n < 1/4$ and $n > 1$, laying down the cosmological framework for these two classes.

In conclusion, the primordial Universe represents an extraordinarily rich epoch for theoretical physics, providing a natural laboratory for high-energy processes and posing fundamental challenges that remain unresolved. Among these, the matter-antimatter asymmetry stands out as one of the most significant problems, if not the most, of this era. A collaborative approach that bridges particle physics and gravitational physics has the potential to illuminate this seemingly simple yet impactful issue. The implications of this slight asymmetry are crucial, not only for the emergence of our existence but also for the evolution of the Universe as we observe it today. The application of modified gravity within the frameworks of two well-established particle physics mechanisms, Electroweak Baryogenesis and Baryogenesis via Grand Unified Theories, has yielded promising results. EWB, in particular, benefited from a significant relaxation of its most stringent constraints, while GUT baryogenesis also showed positive developments. Moreover, modified gravity has proven effective when integrated into the Gravitational Baryogenesis mechanism, where gravity itself plays a central role in generating the baryon asymmetry. This approach has shown fruitful outcomes, especially within a specific model that can be interpreted as a slight deviation from General Relativity in the cosmological context. Hence, modified gravity can be a viable solution to the long last baryonic asymmetry of our Universe.

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