Benemérita Universidad Autónoma de Puebla

Facultad de Ciencias Físico Matemáticas

Transition amplitudes in quantum cosmology

Thesis presented to

Posgrado en Física Aplicada

in partial fulfillment of the requirement for the degree

DOCTOR EN CIENCIAS

by

Jorge Hernández Aguilar

Thesis Advisors

Dr. Cupatitzio Ramírez Romero
Dr. Héctor Hugo García Compéan

Puebla Pue.
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Abstract

In this thesis we present a rigorous examination of vacuum transition probabilities between two minima of a scalar field potential within the framework of quantum cosmology, employing a Lorentzian formalism. The research explicitly incorporates quantum corrections through a Wentzel-Kramers-Brillouin (WKB) approximation to the Wheeler-DeWitt equation, extending the analysis to General Relativity in $(2+1)$ and $(3+1)$ and modified $f(R)$ gravity, offering new insights into the initial conditions of the universe

First we establish the mathematical and conceptual foundations of the research. We provides an introduction to the canonical quantization of gravity, detailing the Arnowitt-Deser-Misner (ADM) formalism and the construction of the Minisuperspace, which leads to the derivation of the Wheeler-DeWitt equation. Additionally, we discuss the conceptual challenges associated with quantum cosmology, such as the Problem of Time and examine the boundary condition proposals essential for the tunneling phenomena, alongside an introduction to the fundamental properties of modified $f(R)$ gravity theories.

Then we develop the general formalism for calculating vacuum transition probabilities. It introduces a method to compute these probabilities for any Minisuperspace model characterized by a Hamiltonian constraint quadratic in the momenta. A key contribution of this formalism is the systematic incorporation of higher-order terms in the semiclassical expansion, enabling the calculation of quantum corrections to the transition amplitudes.

Subsequently, we apply the extended formalism to a $(2+1)$ dimensional gravity model, serving as a theoretical laboratory to explore the implications of metric functions factorization within the Hamiltonian constraint. Transition amplitudes are computed up to the second order in the semiclassical expansion for Friedmann-Lemaître-Robertson-Walker (FLRW) metrics with zero and positive curvature, as well as for anisotropic Bianchi Type I and Type III metrics. Then we extend the analysis to the physically relevant $(3+1)$ dimensional General Relativity. We investigates transition probabilities for flat and closed FLRW metrics, as well as homogeneous anisotropic geometries, specifically Bianchi Type III and Kantowski-Sachs metrics. A significant finding in these chapters is that the inclusion of quantum corrections modifies the transition probabilities in the ultraviolet regime, suggesting a potential resolution to the initial singularity where the universe emerges with a non zero scale factor.

Then we broaden the scope of the investigation to include $f(R)$ modified gravity. The formalism is applied to power-law models, defined by $f(R) = R^{1+n}$, and the Starobinsky model. The analysis considers two distinct approaches: one that assumes a constant Ricci scalar to simplify the derivation of general behaviors, and a more general approach that relaxes this constraint to capture the full effects of the modified gravity sector.

List of publications

The research conducted during the course of this doctoral thesis has resulted in the following list of publications and conference presentations.

- H. García-Compeán, **J. Hernández-Aguilar**, D. Mata-Pacheco and C. Ramírez, "Effects of quantum corrections to Lorentzian vacuum transitions in the presence of gravity," Class. Quant. Grav. **42**, no.2, 025018 (2025) doi:10.1088/1361-6382/ad9fcc [arXiv:2406.13845 [gr-qc]].
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Introduction

A classical field theory may be delineated through the application of a variational principle. For General Relativity, the metric tensor $g^{\mu\nu}$ is considered the fundamental dynamic field variable that describes the gravitational field. General Relativity constitutes the theory that establishes the relationship between the local distribution of mass-energy and the geometry of spacetime. The successful establishment of General Relativity as the theory of the gravitational field is primarily due to the experimental verification of its predictions, which include the perihelion precession of Mercury, the deflection of light by massive objects, gravitational redshift, and, most recently, the observation of gravitational waves originating from the collision of two black holes by the LIGO and Virgo collaborations [1]. The theory, however, inherently predicts its own breakdown due to the inevitable occurrence of singularities within spacetime. The most prominent examples of such singularities are the Big Bang singularity found in the homogeneous and isotropic Friedmann models and the singularity at the center of the spherically symmetric Schwarzschild black hole. These singularities are not merely consequences of the symmetric nature of these solutions. Indeed, the singularity theorems first proven by Hawking and Penrose [2,3] establish that solutions to the Einstein field equations generically possess singularities under rather general assumptions.

Shortly after Einstein published his theory of General Relativity, the scientific community commenced investigation into its cosmological implications. Einstein himself proposed a static universe model. Certain cosmological solutions for the vacuum field equations were derived and studied in [4]. Subsequently, Friedmann abandoned the static universe assumption, allowing the spatial volume to be dynamic while maintaining spatial homogeneity and isotropy. The identical model was independently studied by Lemaitre. Robertson and Walker, demonstrated that the line elements considered up to that point are the only forms compatible with spatial homogeneity and isotropy in $3+1$ dimensions. These models are presently recognized as the Friedmann-Lemaitre-Robertson-Walker (FLRW) models [5].

Besides, Hubble, states the expansion of the Universe, rendered Einstein's static universe model observationally unsustainable. Simultaneously, this discovery affirmed the physical relevance of the FLRW models. Currently, the standard model of cosmology [6] offers a highly consistent description of the Universe's history. The FLRW models are among the simplest solutions to the Einstein field equations, with this simplicity arising from the assumptions of homogeneity and isotropy. The near-isotropy of the Cosmic Microwave Background (CMB), combined with the fundamental result of Ehlers, Geren, and Sachs [7], suggests that the Universe is approximately FLRW at late times. Nevertheless, Wald [8] demonstrated that certain classes of spatially homogeneous models tend to isotropize at late times if a positive cosmological constant is present in the Einstein field equations. This suggests that an inflationary epoch could, in principle, eliminate anisotropies. Consequently, anisotropic models may still be relevant for describing the physics of the early Universe [9]. In addition, there are also some recent experimental studies that suggest that such metrics may be important for the description of our universe even at the present epoch as well [10,11]

At cosmological scales, phenomena lacking a satisfactory explanation are observed, collectively referred to as "dark" matter and energy. Conversely, at microscopic scales, in the vicinity of points that appear as singularities in the classical theory, where matter densities are such that the de Broglie wavelength of a certain mass is of the order of or smaller than the corresponding

Schwarzschild radius, a quantum behavior of the gravitational interaction is expected; specifically, the measurement of distances is subject to quantum fluctuations [12]. The theory describing this behavior must be consistent with the quantum theory and is known as quantum gravitation or the quantum theory of General Relativity. This type of singularity arises in the black hole solutions of Einstein's theory and in cosmology at the beginning of the universe. Moreover, elementary particle physics and cosmology impose constraints on these theories, and no quantum gravitation theories that satisfactorily meet these constraints have yet been formulated [13]. Cosmology studies the evolution of the universe; since it is a closed system, it cannot be stated with certainty to what extent quantum theory must be used for its description, although there are no restrictions in principle [14]. In the context of a quantum theory, the Hamiltonian formulation of the General Relativity is typically utilized [15–17], giving rise to the framework known as quantum cosmology (for a general introduction to the subject of quantum cosmology see [18–22]). Following Dirac's formalism, also known for general relativity as the Arnowitt, Deser and Misner (ADM) formalism [23, 24], the classical Hamiltonian and momentum constraints of a gravitational system are quantized using the Dirac prescription. This leads to a set of constraints on a wave function for the universe, the central object of this framework. When dealing with homogeneous metrics, the information is encoded in the equation resulting from the Hamiltonian constraint. At the quantum level, this constraint is regarded as a Hamiltonian differential operator acting on a wave function defined on the Superspace. Superspace is given by the space of equivalence classes of metrics and matter configurations, modulo the symmetries of the theory, particularly diffeomorphisms [25]; this equation is called the Wheeler-De Witt (WDW) equation [15, 26]. Consistent with the precepts of quantum mechanics, the modulus squared of the wave functions must yield the corresponding probability density for the universe to be found in a certain configuration, and observables are subject to quantum fluctuations. A characteristic feature of General Relativity is that, due to the invariance under time reparameterizations and the fact that the universe is a closed system, the quantum description in the aforementioned formulation is time-independent. Time must therefore emerge from the internal structure of the universe [27].

Furthermore, the classical solutions of General Relativity predict only local properties, and the corresponding spacetimes may possess diverse topologies, as is the case for black holes, such as singularities and wormholes [5]. Consequently, Superspace must contain both the permissible metrics and matter configurations, as well as the allowable topologies, although little is known in this direction. One approach to simplify these studies is through the Minisuperspace formulation, in which the large-scale structure of the universe is considered, and inhomogeneities are neglected, rendering the metric homogeneous. This reduces the problem from a field theory problem to a mechanical one with a finite number of degrees of freedom. In its simplest versions, quantum cosmology does not consider the possibility of non trivial topologies, but the inclusion of different topologies in Superspace opens the possibility of discriminating between them via the corresponding probabilities, which could be obtained from the wave function of the universe. This has been achieved in simple cases, such as theories in two and three dimensions [28, 29], where the degrees of freedom are topological, and the transition probability via tunneling between them can be calculated [29].

In this regard, the phenomenon of vacuum decay represents one of the most intriguing aspects of quantum field theory, with profound implications for particle physics and cosmology. In the canonical approach to quantum gravity, it is thought to provide the description for the birth of our universe. In a general field theory scenario, a scalar field potential containing two local minima of different values separated by a barrier allows for a transition between the two minima via quantum tunnelling. This is called a vacuum transition (analogously, the two minima can also be described by two different values of the cosmological constant). The theoretical framework for understanding false vacuum decay was established in the seminal works of Coleman and Callan [30, 31], who developed the semiclassical instanton method to calculate decay rates. In this formalism, the transition proceeds through the nucleation of true vacuum bubbles (the global minimum) on a false vacuum background, with the decay rate determined by the Euclidean action of a critical bubble configuration known as the bounce solution. The recognition that gravity can significantly influence vacuum transitions led to extensions of the theory. Coleman and De Luccia [32] incorporated gravitational effects, revealing that gravity generally suppresses tunnelling rates. This work, later expanded by Parke [33], established the foundation for understanding vacuum transitions in cosmological contexts. Over the years, many new results have been explored using these Euclidean techniques (see for example [34–43]).

On the other hand, an alternative description to the path integral approach of vacuum decay (for a general review see [44]), can be described by employing a Hamiltonian formalism as mentioned above. One important feature of this formalism is that it does not rely on a Wick rotation; thus, it is a purely Lorentzian method, what means that is possible to study the transition probabilities without requiring any Wick rotation whereas in the Euclidean path integral approach an analytic continuation is required in order to describe the universe after nucleation which may be a relevant limitation. This enables the direct calculation of transition probabilities within the original Lorentzian spacetime framework. The interpretation of this wave function turned out to be very troublesome, since in a cosmological setting describing the entire universe, there is no notion of an external observer (see for example [45, 46] for recent proposals). However, the squared ratio of two solutions of the WDW equation can be interpreted as the conditional probability between two configurations. Using this interpretation, vacuum transition probabilities have been explored in the Lorentzian formalism. Fischler, Morgan and Polchinski studied the transition between two values of the cosmological constant in [47, 48]. Such results were generalized in [49], which examined quantum transitions between Minkowski and de Sitter spacetimes; one important feature of the Lorentzian formalism is that the final state can be a closed universe, contrary to the results obtained with the Euclidean path integral. Later, the inclusion of a scalar field was studied in [50], investigating whether transitions lead to open or closed universe configurations. These approaches have been extended to anisotropic universes [51], alternative gravity theories such as Hořava-Lifshitz gravity [52], and frameworks incorporating generalized uncertainty principles [53]. All these studies provide results only at the semiclassical level. One limitation of this formalism when dealing with the scalar field is that there is not a concrete description of bubble nucleation, however the transition probabilities obtained can be interpreted as probability distributions of creating universes with a given size by vacuum decay, as a generalization of the standard tunnelling from nothing scenario. On the other hand, it is natural to cosider the incorporation of quantum corrections to the transition probabilities. In the Euclidean formalism this issue is troublesome due to the appearance of a negative mode problem that may spoil the semiclassical approximation [54–59]. The Lorentzian formalism, however, employs a semiclassical expansion in the form of a WKB proposal. In this way, the quantum corrections are incorporated by considering the higher-order terms in the $\hbar$ expansion. It has been shown for field theory that the first quantum correction computed in this form indeed coincides with the 1-loop contribution of the Euclidean formalism [60]. For recent developments regarding the incorporation of quantum gravity corrections employing the WDW equation see also [61–65].

Also, recent advances in calculational techniques have further enhanced the capacity to study vacuum transitions. In [66, 67] the calculation of tunneling actions was reformulated as an elementary variational problem. Building upon this, [68–71] developed general methods for finding scalar potentials with exactly solvable decay at the semiclassical level. Furthermore, the holographic interpretation of these transitions has also been explored [72–75]. These developments have been complemented by studies examining specific aspects of the tunneling process [76–80], non-minimal couplings [81], and applications to Lorentzian path integrals [82]. In this way, in this thesis quantum corrections are incorporated by considering the higher-order terms in the WKB expansion. Obtaining analytical expressions for transition probabilities up to second-order quantum corrections in both homogeneous isotropic and anisotropic cosmological models.

Further, just as quantum corrections were incorporated into probability calculations, modifications to the gravitational sector warrant equal consideration. The study of vacuum decay in modified gravity theories represents a natural and necessary extension of the original Coleman-

De Luccia framework. Higher-order curvature terms, which generically emerge in effective field theories of gravity, play crucial roles in various cosmological contexts (See [83–87]). In this context, [39] investigates the effects of the Gauss-Bonnet term on vacuum decay, demonstrating that higher-order curvature corrections can significantly modify tunneling rates. This analysis was subsequently extended to examine vacuum transitions with the Gauss-Bonnet term in arbitrary dimensions [88]. Meanwhile, [89] explores how higher-derivative gravity theories can be probed through tunneling phenomena. As well, in [90, 91] have systematically investigated vacuum decay in quadratic gravity, examining both massless and massive cases, and established new bounds on vacuum decay rates in de Sitter space [92].

Among the various modified gravity theories [93, 94], $f(R)$ gravity occupies a particularly prominent position due to its theoretical frame and phenomenological relevance. The $f(R)$ formalism [95–97] generalizes the Einstein-Hilbert action by replacing the Ricci scalar R with an arbitrary function $f(R)$. This class of theories has demonstrated remarkable success in addressing outstanding problems in cosmology. Particularly, in [98] is examined the classical and quantum cosmology of the Starobinsky inflationary model, an $f(R)$ theory that provides a compelling mechanism for early universe inflation. In [99] $f(R)$ gravity has been employed to connect early and late universe dynamics , offering unified descriptions of inflation and late-time cosmic acceleration. Moreover, for example in [100] and [101] is demonstrated that exponential and power-law inflation can be realized within $f(R)$ frameworks.

The consideration of $f(R)$ gravity in vacuum decay problems is motivated by several compelling considerations. First, $f(R)$ modifications represent the simplest extension of general relativity that incorporates higher-order curvature effects without pathologies such as the ghost instabilities, making them ideal testing grounds for understanding how modified gravity influences quantum tunneling processes. Second, the additional scalar degree of freedom present in $f(R)$ theories, which emerges from the higher-order curvature terms, can couple to matter fields in non-trivial ways that affect vacuum stability and transition rates. Third, $f(R)$ theories admit consistent quantum mechanical treatments, as demonstrated by studies of the Wheeler-DeWitt equation in $f(R)$ cosmology [102–104], ensuring that quantum aspects of vacuum transitions can be properly addressed within these frameworks. In this way, Salehian and Firouzjahi [105] performed pioneering work on vacuum decay and bubble nucleation in $f(R)$ gravity, deriving modified bounce equations and demonstrating that the functional dependency on the Ricci scalar significantly impacts decay rates and critical bubble configurations.

This thesis presents a study of vacuum transition probabilities between two minima of a scalar field potential employing a Lorentzian formalism in the presence of gravity and modified gravity. explicitly incorporating quantum corrections. The organization of the work is as follows:

In Chapter 1, we establish the mathematical and conceptual foundations of the research. We begin with an introduction to quantum cosmology, addressing the fundamental principles of the ADM formalism and providing an exposition of the minisuperspace concept, which culminates in the derivation of the Wheeler-DeWitt equation. Furthermore, the chapter examines the implications of the canonical treatment of General Relativity, specifically the Problem of Time and the boundary conditions proposals, thereby establishing the context in which tunneling phenomena arise within quantum cosmology. Furthermore, the general features of modified $f(R)$ gravity theories are presented, which are addressed within the framework of this work.

Subsequently, in Chapter 2, we present the general formalism for addressing vacuum transition probabilities between two minima of a scalar field potential, utilizing the semiclassical Wentzel-Kramers-Brillouin (WKB) approximation to the Wheeler-DeWitt equation within a Lorentzian framework. We first introduce a general method to compute these probabilities for any model on minisuperspace by considering a general Hamiltonian constraint defined by quadratic terms in the momenta. This method systematically incorporates higher-order terms of the semiclassical expansion, thereby allowing for the inclusion of quantum corrections to the transition probabilities.

In Chapter 3, we apply the extended general formalism to a $(2 + 1)$-dimensional gravity toy model, thereby exploring the method with a specific focus on the implications of metric function factorization within the Hamiltonian constraint. We compute the transition amplitudes up to the second order in the semiclassical expansion for FLRW metrics characterized by cero and positive curvature. Furthermore, we investigate anisotropic geometries, specifically the Bianchi Type I and Type III metrics. We demonstrate that, at the leading order of the WKB expansion, certain models yield results analogous to those previously reported in the literature for the corresponding $(3+1)$ dimensional metrics. However, we wish to emphasize that the specific calculation of transition amplitudes and tunneling probabilities between distinct minima of a scalar field potential within the $(2+1)$ dimensional framework has not been previously addressed.

Motivated by the results obtained for the $(2+1)$ dimensional case, in Chapter 4, we employ the general formalism established herein to compute vacuum transition probabilities within $(3+1)$-dimensional General Relativity. We commence with an analysis of the FLRW metric, considering both positive and zero spatial curvatures. Subsequently, we extend this to investigate transition probabilities in the context of homogeneous anisotropic geometries, specifically the Bianchi Type III and Kantowski-Sachs metrics, to examine the implications of anisotropy on the quantum corrections. In this instance, it is observed that the inclusion of quantum corrections modifies the transition probabilities in the ultraviolet regime, resulting in their vanishing as the scale factor approaches zero. Under an appropriate physical interpretation, this behavior presents a plausible resolution to the initial singularity; specifically, if the universe originates via a vacuum transition within this framework, it is predicted to emerge free of a singularity. The results presented in this chapter were first published in [161].

Given that the applicability of the proposed method is not restricted to General Relativity, requiring only that the Hamiltonian of the model be quadratic in the momenta, Chapter 5 extends the analysis to include $f(R)$ modified gravity alongside the evaluation of quantum corrections. Specifically, we reexamine the metrics discussed in the preceding chapter within the context of power-law $f(R)$ models and the Starobinsky model. We consider two distinct approaches. In the first, the Ricci scalar is treated as a constant; this assumption yields simplifications that facilitate the analysis of the probabilities and permits the determination of their general behavior, analogous to the results presented in the preceding chapter. The second approach proceeds without this condition, thereby modifying the associated dependencies. However, the inclusion of $f(R)$ gravity entails specific limitations, which are addressed within this chapter. These results are currently being prepared for publication.

Finally, in Chapter 6, we present our concluding remarks.

Chapter 1

Preliminaries

All known interactions, excluding gravity, are accurately described by quantum field theory. Indeed, quantum theory appears to provide a universal framework for describing nature. Gravity, however, has thus far resisted all attempts to formulate it within a quantum framework. Furthermore, quantum gravitational effects currently remain beyond the reach of experimental and observational verification. There is a general consensus that the issue of singularities will ultimately be resolved within a quantum theory of gravity. Attempts to formulate a quantum theory of gravity proceed primarily from two directions. One approach proposes starting from a classical theory of gravity, such as General Relativity or an alternative modification thereof, and applying canonical quantization rules to yield Quantum General Relativity or Quantum Geometrodynamics. The second approach attempts to formulate a unified theory of all interactions, aiming to recover Quantum General Relativity in an appropriate limit.

The initial attempts to directly quantize General Relativity were undertaken by DeWitt in the seminal works [15–17], where [15] addresses the canonical approach, and [16, 17] deal with the covariant approach. The canonical approach shall be followed here, where the core concept of Quantum Cosmology is to apply standard quantization procedures to a minisuperspace model. This idea was originally implemented in [15]. The focus will be on the Wheeler-DeWitt equation for the minisuperspace, which is the equation obtained by applying the Dirac quantization procedure to the symmetry-reduced model. The Wheeler-DeWitt equation in minisuperspace is no longer a functional partial differential equation but reduces to an ordinary partial differential equation. In essence, following canonical quantization, the problem reduces from one of quantum field theory to one of quantum mechanics. This chapter addresses the general principles of the canonical formulation of General Relativity to obtain the WDW equation and its consequences, thereby establishing the initial framework for calculating transition probabilities.

1.1 Dirac-Bergmann Algorithm

The standard methodology of Hamiltonian mechanics [106–109] commences with a system characterized by n spatial coordinates, denoted as $q^1, \ldots, q^n$. Given a Lagrangian $\mathcal{L}\left(q^1, \ldots, q^n, \dot{q}^1, \ldots, \dot{q}^n\right)$, the Euler-Lagrange equations yield the n equations of motion

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathcal{L}}{\partial \dot{q}^i} = \frac{\partial \mathcal{L}}{\partial q^i} \quad i = 1, \ldots, n. \tag{1.1}$$

To transition to the Hamiltonian formalism, a Legendre transformation is performed, defining the conjugate momenta p_i as

$$p_i := \frac{\partial \mathcal{L}}{\partial \dot{q}^i}. \tag{1.2}$$

The system is subsequently described within a $2n$-dimensional phase space using the coordinates $q^1, \ldots, q^n, p_1, \ldots, p_n$. The Hamiltonian $\mathcal{H}$ is defined through the relation:

$$\mathcal{H} := p_i \dot{q}^i - \mathcal{L}. \tag{1.3}$$

The corresponding equations of motion are provided by Hamilton's equations:

$$\dot{q}^i = \{\mathcal{H}, p_i\} \quad \text{and} \quad \dot{p}_i = \{\mathcal{H}, q_i\}, \tag{1.4}$$

where

$$\{f, g\} = \frac{\partial f}{\partial q^i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q^i} \tag{1.5}$$

denotes the Poisson bracket. The Lagrangian and Hamiltonian formalisms are fundamentally equivalent; however, the inversion of the Legendre transform may be obstructed. Specifically, if the Hessian matrix $(\partial^2 \mathcal{L}/\partial \dot{q}^i \partial \dot{q}^j)$ is singular, the momenta cannot be expressed as invertible functions of the coordinate derivatives. This scenario necessarily introduces constraints,

$$\varphi_k\left(q^i, p_i\right) = 0, \tag{1.6}$$

meaning that the system is restricted to a physically allowable submanifold of the phase space. Such functions φ_k, which are immediately found to vanish based on the definition of the momenta, are termed primary constraints. The notation of weak equality, $\varphi_k \approx 0$, is employed to signify that this condition holds only for physically permissible events within the constrained phase space, rather than across the entire $2n$-dimensional coordinate space.

Consequently, the standard Hamiltonian formalism is incomplete without incorporating constraint information. To address this deficiency, the Hamiltonian can be modified via the introduction of Lagrange multipliers λ^k associated with the constraints φ_k

$$\widetilde{\mathcal{H}} = \mathcal{H} + \sum_k \lambda^k \varphi_k. \tag{1.7}$$

It is noted that $\mathcal{H}$ and $\widetilde{\mathcal{H}}$ are weakly equal. From this modified Hamiltonian, the Euler-Lagrange equation with respect to the variable λ^k directly yields the equation of motion $\varphi_k = 0$, thereby integrating the constraint into the dynamics. The modified Hamiltonian also provides new Hamilton's equations for an arbitrary function $f\left(q^i, p_i\right)$

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \{\mathcal{H}, f\} + \lambda^k \{\varphi_k, f\}. \tag{1.8}$$

This modified approach allows for the inversion of the transform, yielding

$$\dot{q}^i = \frac{\partial \mathcal{H}}{\partial p_i} + \lambda^j \frac{\partial \varphi_j}{\partial p_k}. \tag{1.9}$$

In exchange for restoring invertibility, the introduction of additional constraints may be required. Since φ_k must vanish, its time derivative must also weakly vanish

$$0 \approx \dot{\varphi}_k = \{\mathcal{H}, \varphi_k\} + \lambda^\ell \{\varphi_\ell, \varphi_k\}. \tag{1.10}$$

In most instances, this imposes a restriction on the multipliers λ^ℓ. However, if the right-hand side is found to be independent of λ^ℓ and non-trivial, a new constraint on the original coordinates, $\psi(p, q) \approx 0$, emerges. Thus, a family of constraints ψ_k may be derived from certain φ_k. New Lagrange multipliers can then be added to the Hamiltonian, and Equation (1.10) imposed for the ψ constraints to obtain further constraints, a process that continues iteratively for each newly derived constraint. This procedure generates a collection of *secondary constraints*, $\psi_k \approx 0$. These are designated as secondary constraints because their origin lies in the application of Hamilton's equations to other constraints, rather than solely in the algebraic definition of the coordinates.

1.2 The ADM Formalism

In classical field theory [110–112], one studies a Lagrangian density whose coordinate functions are fields permeating spacetime (the usual Lagrangian is the integral of the density over all of space). When we solve the equations of motion, they will describe the physical field configuration our theory predicts. The natural choice of field in our theory of gravity is just the tensor field $g_{\mu\nu}$ for which solution of the Einstein vacuum equations extremizes the Einstein-Hilbert Action,

$$S = \int \mathcal{L}_G \, \mathrm{d}^4 x \quad \text{where} \quad \mathcal{L}_G = \frac{1}{2}\sqrt{-g}R \tag{1.11}$$

is the Lagrangian density of our system In natural units ($c = 1$, $8\pi G = 1$). We will want the time variable to be explicit when we consider the Hamiltonian picture, this requires the $3+1$ decomposition of the metric in which the spatial components of the metric serve as the dynamic degrees of freedom. In geometrical language, this can be viewed as a decomposition of the four-dimensional manifold $\mathcal{M}$, which is assumed to be globally hyperbolic and endowed with a Lorentzian metric. A global causal time function $\tau \in \mathcal{R}$ can then be chosen, and $\mathcal{M}$ can be foliated into Cauchy hypersurfaces Σ_τ, such that the spacetime topology results in $\mathcal{M} \to \mathcal{R} \times \Sigma$, where Σ denotes a three-dimensional hypersurface of arbitrary, space-like topology. It is important to emphasize that the choice of the global time function does not introduce time as an absolute quantity and does not lead to a preferred foliation, as is guaranteed by the diffeomorphism invariance of the theory. Therefore, all foliations are physically equivalent. So we may rewrite the Lagrangian density as

$$\begin{aligned} \mathcal{L}_{ADM} &= \frac{1}{2}N\sqrt{h}\left({}^3R + K_{ij}K^{ij} - K^2\right) \\ &= \frac{1}{2}N\sqrt{h}\left[{}^3R + \left(h^{ir}h^{js} - h^{ij}h^{rs}\right)K_{ij}K_{rs}\right] \end{aligned} \tag{1.12}$$

where $K_{ij} = \frac{1}{2N}\left(\partial_i N_j + \partial_j N_i - \partial_0 h_{ij}\right)$ is the extrinsic curvature, $K = h^{ij}K_{ij}$ is its trace, and ${}^3R$ is the intrinsic curvature of the three-dimensional slice. We choose the fields of our field theory to be the 3-metric components h_{ij} and our lapse and shift vectors N, and N^i. For every fixed time τ, this defines ten independent scalar field components just as for our original 4-metric g. Note that K is independent of derivatives of lapse and shifts, so we have that the conjugate momenta associated to N and each N^i are constrained to vanish, in this way

$$\begin{aligned} \pi &:= \frac{\partial \mathcal{L}_{ADM}}{\partial\left(\partial_\tau N\right)} \approx 0 \\ \pi_k &:= \frac{\partial \mathcal{L}_{ADM}}{\partial\left(\partial_\tau N^k\right)} \approx 0 \end{aligned} \tag{1.13}$$

These are primary constraints in our system. The other conjugate momenta associated to components of h are

$$\pi^{ij} := \frac{\partial \mathcal{L}_{ADM}}{\partial\left(\partial_\tau h_{ij}\right)} \tag{1.14}$$

Considering the useful relation,

$$K_{ij} = \frac{1}{2N}\left(\partial_\tau h_{ij} - {}^3\nabla_i N_j - {}^3\nabla_j N_i\right) \tag{1.15}$$

easily follows that,

$$\pi^{ij} = \frac{1}{2}\sqrt{h}\left(K^{ij} - Kh^{ij}\right) = \frac{1}{2}\sqrt{h}\left(h^{ir}h^{js} - h^{ij}h^{rs}\right)K_{rs}. \tag{1.16}$$

Additionaly, If we define the tensor

$$G_{ijrs} = \frac{1}{2\sqrt{h}}\left(h_{ir}h_{js} + h_{is}h_{jr} - h_{ij}h_{rs}\right) \tag{1.17}$$

known as Wheeler's metric, we may rewrite the Lagrangian density as

$$\mathcal{L}_{ADM} = \frac{1}{2} N\sqrt{h}\,^3R + 2NG_{ijrs}\pi^{rs}\pi^{ij} \tag{1.18}$$

By the standard procedure (remembering our constraints and the Lagrange multipliers), we obtain the Hamiltonian density,

$$\mathcal{H}_{ADM} = \lambda\pi + \lambda^i\pi_i + N^k\mathcal{H}_k + N\mathcal{H} + 2^3\nabla_i\left(\pi^{ij}N^k k_{kj}\right). \tag{1.19}$$

where,

$$\mathcal{H} := 2G_{ijrs}\pi^{rs}\pi^{ij} - \frac{1}{2}\sqrt{h}\,^3R \tag{1.20}$$

and

$$\mathcal{H}_k := -2h_{kj}\,^3\nabla_i\pi^{ij} \tag{1.21}$$

are called the superHamiltonian and supermomenta respectively. We can ignore the last term of (1.19) since it is a total derivative and so when we integrate it in the action it vanishes on any compact interval by Stoke's theorem. On the other hand, we require from the constraints that

$$\begin{aligned} 0 &\approx \{\pi, \mathcal{H}_{ADM}\} = -\mathcal{H} \\ 0 &\approx \{\pi_k, \mathcal{H}_{ADM}\} = -\mathcal{H}_k \end{aligned} \tag{1.22}$$

We conclude that the Hamiltonian density of (1.19) is a sum of quantities which weakly vanish and so we deduce that it weakly vanishes as well,

$$\mathcal{H}_{ADM} \approx 0. \tag{1.23}$$

The superHamiltonian as given in equation (1.20) provides the evolution of the system. The supermomentum constraint (1.21) defines the configurational space of the canonical gravity that it is the infinite dimensional space of all the possible geometries [19, 113].

1.3 Superspace and Minisuperspace

The Superspace is the configuration space upon which the wave function of the Universe is defined. To construct this space, one begins by considering the configuration space containing all Riemannian 3-metrics h_{ij} and matter field configurations $\Phi(x)$ on a spatial hypersurface Σ, such that

$$\mathrm{Riem}(\Sigma) = \{h_{ij}(x), \Phi(x) | x \in \Sigma\}. \tag{1.24}$$

If a diffeomorphism can relate a set of configurations, these configurations must possess the same intrinsic geometry and are considered physically equivalent. One then proceeds to partition this space into equivalence classes, where two configurations belong to the same class if they are related by a diffeomorphism. Superspace is thus defined as the following quotient

$$\mathcal{S}(\Sigma) = \mathrm{Riem}(\Sigma)/\mathrm{Diff}_0(\Sigma), \tag{1.25}$$

where the subscript 0 signifies that only those diffeomorphisms connected to the identity are considered. Discussing Superspace, which is infinite-dimensional, is non-trivial, and it is generally not possible to make exact statements about it. However, a common approach is to focus on a finite number of degrees of freedom $x^\alpha(t)$. By doing this, one can effect a dimensional reduction of Superspace, creating a Minisuperspace which is finite-dimensional and can be approached using isotropic and homogeneous 3-surfaces [15]. There is no definitive certainty that Minisuperspace constitutes a systematic approximation to the complete theory. Arguments regarding the validity of this finite-dimensional Minisuperspace approximation are presented in reference [114]. In this reduced space, the shift vector is set to $N^i = 0$, and the lapse function is homogeneous, such that $N = N(t)$. Within this context, these systems are frequently referred to as minisuperspace models, and this terminology shall be adopted herein.

1.4 Wheeler-DeWitt Equation

In order to quantize, we need to promote the coordinates and momenta to operators on a space of states. In quantum mechanics, the state space is the Hilbert space of L^2 functions on the configuration space. The same is true in quantum field theory, except the configuration space is infinite dimensional, corresponding to the value of the field at every point in spacetime. When we quantize, the Hilbert space is Fock space, complex valued functionals on the space of all field configurations [115, 116].

For us, the configuration space is all possible spacetime metrics h and values for the lapse and shift vectors. The quantized space of states should be the space of L^2 functionals on this space. One can informally think of this like traditional quantum mechanics which describe particles by wavefunctions that represent a probability distribution on possible positions of the particle; instead of the universe being composed of a single space time metric, it is a delocalized combination of many different metrics. This is an informal description of the idea of quantum foam, in which the local structure of space is not fixed but a bubbling quantum superposition Ψ. The procedure for giving our space of metrics and Lebesgue measure and hence a proper L^2 Hilbert space structure on states is not currently known. Nevertheless, we persist, treating the states and operators as purely formal expressions.

As in quantum field theory, we will make our fields of interest and their conjugate momenta into operators on our Hilbert space, denoted with a hat over the relevant classical quantity, and in analogy with quantum mechanics, in a coordinate basis, we may consider our coordinate operators as multiplication operators and our momenta operators as functional derivatives acting on functionals $\Psi\left[h_{ij}, N^i, N\right]$

$$
\begin{aligned}
\widehat{h}_{ij}(x)(\Psi) = h_{ij}(x)\Psi \quad \widehat{\pi}^{ij}(x)\Psi = -i\frac{\delta\Psi}{\delta h_{ij}(x)}\\
\widehat{N}(x)(\Psi) = N(x)\Psi \quad \widehat{\pi}(x)\Psi = -i\frac{\delta\Psi}{\delta N(x)}\\
\widehat{N}^i(x)(\Psi) = N^i(x)\Psi \quad \widehat{\pi}_i(x)\Psi = -i\frac{\delta\Psi}{\delta N^i(x)}
\end{aligned}
\tag{1.26}
$$

Given our total space of states, the constraints we found in the ADM theory will tell us that only certain states are physically allowable. This will restrict us to some subspace on which constraint equations are satisfied. Recall we had primary constraints $\pi \approx \pi_k \approx 0$ and so for arbitrary physical state ψ we must have that,

$$
-i\frac{\delta\Psi}{\delta N} = -i\frac{\delta\Psi}{\delta N^k} = 0 \tag{1.27}
$$

In particular, $\Psi = \Psi\left[h_{ij}\right]$ must be a functional of the three-metrics alone, independent of lapse and shift vectors. We also found that the whole Hamiltonian was constrained to vanish via our supermomentum and superHamiltonian. Imposing the vanishing of the components of the supermomentum gives

$$
\widehat{\mathcal{H}}_i\Psi = -2h_{ik}{}^3\nabla_j\left(\frac{\delta\Psi}{\delta h_{jk}(x)}\right) = 0 \tag{1.28}
$$

The significance of the momentum constraint was first identified and demonstrated by Peter Higgs in [117]. From the above equation, it follows that the theory is invariant under three-dimensional diffeomorphisms. To demonstrate this, consider an infinitesimal coordinate transformation

$$
x_i \to x_i' = x_i - \eta_i, \tag{1.29}
$$

under which the wave functional transforms as

$$
\Psi\left[h_{ij} + D_{(i}\eta_{j)}\right] = \Psi\left[h_{ij}\right] + \int \mathrm{d}^3x D_{(i}\eta_{j)}\frac{\delta\Psi}{\delta h_{ij}}. \tag{1.30}
$$

Assuming compact geometries, integration by parts allows the boundary terms to be discarded. The preceding expression is thus rewritten as

$$\Psi\left[h_{ij}+D_{(i}\eta_{j)}\right]=\Psi\left[h_{ij}\right]-\int \mathrm{d}^3x\eta_j D_i\left(\frac{\delta\Psi}{\delta h_{ij}}\right)=\Psi\left[h_{ij}\right]+\frac{1}{2i}\int \mathrm{d}^3x\eta_i\mathcal{H}^i\Psi. \tag{1.31}$$

If the momentum constraint is satisfied, the second term on the right-hand side of the equation vanishes, yielding

$$\Psi\left[h_{ij}+D_{(i}\eta_{j)}\right]=\Psi\left[h_{ij}\right], \tag{1.32}$$

thereby proving the invariance. When the constraints are taken *on-shell*, the integrand and consequently the Hamiltonian vanish. This presents a problem, as in quantum mechanics, the Hamiltonian is responsible for generating time translations, which are interpreted as the flow of time. A vanishing Hamiltonian would thus imply the absence of such a flow. This issue precisely highlights one of the primary difficulties in attempts to construct theories of quantum gravity [118]. Essentially, this conflict arises from the independent and incompatible notions of time inherent in quantum mechanics and general relativity. In quantum mechanics, time is treated as a background parameter with a rigid and absolute flow, external to the system itself. Conversely, in general relativity, time is a coordinate whose flow may depend on the motion and position of the system under consideration. Finding a solution to this dilemma is of paramount importance if one seeks to replace quantum theory and general relativity with a unified framework capable of addressing situations where the effects of both are significant.

Turning our attention to the Hamiltonian constraint, as previously noted, within the minisuperspace approximation, the shift vector vanishes and the lapse function is homogeneous. Consequently, the line element in this space is given by

$$ds^2=-N^2(t)dt^2+h_{ij}(\boldsymbol{x},t)dx^idx^j. \tag{1.33}$$

Now, Let the indices M,N range over the set of independent components of the spatial metric h_{ij}, such that $M,N\in\{h_{11},h_{22},h_{33},h_{12},h_{13},h_{23}\}$. The Wheeler-DeWitt metric may then be expressed as

$$\mathcal{G}_{MN}=\mathcal{G}_{(ij)(kl)}. \tag{1.34}$$

This formulation allows the Hamiltonian constraint to be written as

$$\mathcal{H}=\pi_M\dot{x}^N-\mathcal{L}_{ADM}=N\left[\frac{1}{2}G^{MN}\pi_M\pi_N+\mathcal{V}(x)\right], \tag{1.35}$$

where

$$\mathcal{V}(x)=-\frac{1}{2}{}^3R. \tag{1.36}$$

The preceding expression arises from the Hamiltonian constraint of the full theory, integrated over the spatial hypersurfaces. Thus, if we also consider the coupling of matter, as in the specific case addressed within this thesis, these matter fields would be implicitly contained within the function $\mathcal{V}$. Denoting Φ as the collective symbol for all remaining fields, we can then write the following expression

$$\mathcal{H}=\frac{1}{2}G^{MN}(\Phi)\pi_M\pi_N+\mathcal{V}[\Phi]\approx 0. \tag{1.37}$$

On the other hand, provided that the operator ordering ambiguities are rectified by requiring that the derivatives with respect to the components Φ_M of Φ be covariant with respect to the metric G_{MN}, the replacement $\pi_M\to -i\hbar\frac{\delta}{\delta\Phi^M}$ in the expression (1.37), leading to

$$\mathcal{H}\Psi(\Phi)=\left[-\frac{\hbar^2}{2}G^{MN}(\Phi)\frac{\delta}{\delta\Phi^M}\frac{\delta}{\delta\Phi^N}+\mathcal{V}[\Phi]\right]\Psi[\Phi]=0, \tag{1.38}$$

This is the so-called Wheeler-DeWitt equation, where Ψ is the wave function of the universe and Φ encompasses all minisuperspace coordinates Φ^M, these include the elements of the three-dimensional metric, variables of the matter fields, etc., along with their respective canonically conjugate momenta π_M. Additionally, $\mathcal{V}[\Phi]$ refers to all remaining terms related to 3-curvature and potential terms of matter fields that emerge in the WDW equation. The dynamic content of quantum geometrodynamics is provided by this equation. Unlike the Schrödinger equation, the Wheeler-DeWitt equation is a timeless equation. The usual concept of time only emerges as an approximate notion in the semiclassical limit [113]. Also, we can see the ambiguity of factor ordering in this WDW equation, but there exist natural choices of ordering for which derivative terms become a Laplacian in the supermetric (See [119] and references therein).

Analogous to wave functions in non-relativistic particle mechanics, a probability interpretation is associated with our wave function. Because the Wheeler-DeWitt equation takes a Klein-Gordon form, there exists a conserved current corresponding to

$$J = \frac{i}{2}\left(\Psi\nabla\Psi^* - \Psi^*\nabla\Psi\right). \tag{1.39}$$

While it may seem natural to interpret J as a probability flux, it is not positive definite. For this reason, probabilities constructed from the conserved current J are rejected. Instead, many adopt Hawking's proposal that $\|\Psi[h_{ij}, \Phi, \Sigma]\|^2$ should be interpreted as being proportional to the probability that the Universe contains a 3-surface Σ with metric h_{ij} and matter field Φ. Explicitly, the probability of finding the Universe in a configuration contained within a region $\mathcal{M}$ of our superspace [120] is then

$$P(\mathcal{M}) \propto \int_{\mathcal{M}} \|\Psi\|^2 \cdot 1, \tag{1.40}$$

where 1 denotes the volume element. On the other hand, in quantum field theory, solutions to the Klein-Gordon equation are quantized and become field operators. Following this approach for the Wheeler-DeWitt equation leads to proposals that Ψ should undergo a third quantization and be converted into an operator $\hat{\Psi}$. This operator creates and annihilates universes in the same manner as the familiar ladder operators associated with the Klein-Gordon field create and annihilate particles. The difficulties with this method arise from the fact that we clearly cannot perform measurements on a statistical ensemble of universes in the same way we can with particles. Consequently, it remains unclear how the application of this method could yield measurable probabilities [19, 121, 122]. Conversely, solutions to the Wheeler-DeWitt equation do not inherently define a probability measure; however, they may be utilized to construct a conditional probability framework suitable for physical interpretation [49–51]. In this context, the ratio of the squared moduli of the wave functionals corresponding to distinct configurations (as we will see, two minimia of the scalr field potential) is interpreted as the relative probability of a transition between two states. We will employ this conditional probability approach to investigate vacuum transitions.

1.5 The Problem of Time

The quantum Hamiltonian constraint, as expressed in (1.20), imposes the condition that the operator $\hat{\mathcal{H}}$ annihilates physical states. The Schrödinger equation corresponding to this constraint can be written as

$$\hat{\mathcal{H}}\Psi = i\frac{\partial\Psi}{\partial t} = 0. \tag{1.41}$$

This equation implies the time independence of the wave function Ψ, thereby precluding any notion of quantum evolution within the system. Such pathology suggests that quantum gravity lacks of time evolution, a issue widely recognized as the problem of time [22, 118, 123].

The origin of this issue lies in the fundamental disparity between general relativity and quantum mechanics. In quantum mechanics, time serves as an external, fixed scalar parameter governing the evolution of the system. By contrast, General Relativity treats time as a dynamical entity, rendering the identification of a suitable time parameter problematic in quantum gravitational frameworks. The absence of a well defined temporal structure complicates the interpretation of probability and measurement within quantum theory, unless these concepts are redefined.

To circumvent the problem of time, we must introduce a first order momentum term into the Hamiltonian. At the classical level, one may identify a time coordinate q_M and express the scalar constraint in terms of its conjugate momentum p_M as

$$p_M + H_M = 0, \tag{1.42}$$

where H_M denotes the reduced Hamiltonian. This formulation permits evolution with respect to the time variable q_M, yielding a Schrödinger-like equation of the form

$$\hat{H}_M \Psi = i \frac{d\Psi}{dq_M}. \tag{1.43}$$

The selection of the time variable q_M can be approached in two distinct ways. First, q_M may be chosen from the gravitational configuration space, though this approach restricts quantization to a subset of the gravitational degrees of freedom [124]. Alternatively, the time coordinate q_M may be derived from an external matter field, allowing the gravitational sector of the Hamiltonian to evolve with respect to a time parameter defined by the matter distribution. A notable implementation of this approach involves the use of a fluid, where the monotonic evolution of fluid density serves as a viable time parameter [125,126]. Despite the absence of an explicit time parameter to introduce dynamical evolution into the Wheeler–DeWitt equation, physically meaningful results may still be derived through the conditional probability approach adopted in this thesis.

1.6 Boundary Condition Proposals

The Wheeler-DeWitt equation, when applied as a dynamical theory, requires the imposition of boundary conditions to yield a unique solution describing the observable universe. Analysis centers on two principal proposals: the Vilenkin tunnelling proposal [127] and the Hartle-Hawking no-boundary proposal [128], defining the paths for application of quantum cosmology; the Hartle-Hawking no-boundary proposal and the Vilenkin tunnelling proposal . The Hartle-Hawking (HH) no-boundary proposal posits that the universe has no boundary at the beginning. The wave function is determined by a Euclidean path integral over all compact, positive-definite four-geometries for which the specified three-geometry serves as the only boundary. It is later established [129,130] that different convergent contours are dominated by distinct saddle-points, which lead to different wave functions. The proposal by Hartle and Hawking does not offer guidance in making a choice among these contours. However, it is asserted that there are no preferred contours, but only some that are considered superior to others. The universe is assumed to have originated from a regular Euclidean geometry, subsequently transitioning to a Lorentzian geometry.

The tunnelling proposal, made by Vilenkin, posits that the universe spontaneously nucleated from a vacuum state (characterized by no space, time, or matter) into an inflationary de Sitter spacetime. This concept can be formulated via a path integral over Lorentzian metrics [131,132], where the initial three-geometry is contracted to a single point, contrasting with the HH proposal by not restricting the integration to compact Euclidean geometries. Such that at singular boundaries the wave function of the universe must consist only of outgoing modes. Furthermore, in [133] it is demonstrated that the Wick rotation employed by HH should be performed on the negative time instead of the positive. However, this proposal yields results identical to the Vilenkin proposal, for simple models and is thus commonly classified under the tunneling proposal as well.

Both proposals lead to the paradigm that the universe was created from nothing scenario by a tunnelling event. A common method employed to analyze the oscillatory (classically allowed) regions of the wave function is the WKB approximation, which serves as a common method employed to analyze the oscillatory (classically allowed) regions of the wave function, ensuring that solutions correspond to classical spacetime at large-universe limits. Despite this common conceptual origin, the proposals yield divergent predictions regarding the likelihood of sufficient inflation. Within the minisuperspace framework, the two boundary conditions mentioned lead to a wave function that predicts an inflationary period [134]. The amount of inflation a universe experiences is determined by the initial value of the scalar field, Φ_0. The proposals yield different probability distributions for this initial value. Both proposals have been studied extensively (See for example [122, 135–137]).

1.7 General Features of $f(R)$ Theories

From the perspective of quantum field theory, it is established that General Relativity is described by the propagation of a massless spin-2 particle, known as the graviton. However, within this framework, General Relativity is recognized as a non-renormalizable theory. Consequently, with the aim of obtaining a quantum description of the gravitational field or addressing other pathologies, proposing modifications to it has been of particular interest. Early attempts to develop modified theories of gravity [96, 95, 97] involved introducing higher order invariants into the Einstein-Hilbert action [138, 139]. Subsequently, it was demonstrated that one-loop renormalization required the Einstein-Hilbert action to include higher-order terms in the Ricci scalar R [140]. Moreover, it has been shown that higher-order actions are renormalizable [141]. Furthermore, when considering quantum corrections or working within the framework of string theory, the minimum effective energy of gravitational actions naturally admits higher order curvature invariants. These considerations underscore the interest in modified theories of gravity. However, the significance of these terms is typically restricted to regimes of intense gravitational fields, rendering them negligible at low energies and large scales, such as in the late Universe. Thus, corrections to General Relativity become significant near the Planck scale, and consequently, in the early Universe or in the vicinity of black hole singularities.

An alternative approach to addressing the limitations inherent in GR is to consider that the current description of the gravitational field is incomplete. Following Einstein's proposal of General Relativity and Hilbert's Lagrangian describing it, Kretschmann [142] proposed an action constructed with the scalar $R_{\alpha\eta\gamma\delta}R^{\alpha\eta\gamma\delta}$ instead of the Ricci scalar; this was later known as the Kretschmann scalar

$$S_K = \int_{\mathcal{M}} d^4x\sqrt{-g}R_{\alpha\eta\gamma\delta}R^{\alpha\eta\gamma\delta}. \tag{1.44}$$

Given that the Riemann tensor $R_{\alpha\eta\gamma\delta}$ is the fundamental tensor for gravitation and the Kretschmann scalar is its square, this Lagrangian appears to be a viable option; furthermore, this theory preserves the Bianchi identities. However, the appearance of terms of the form $\nabla_\alpha\nabla_\beta R^\alpha_{(\gamma\delta)}$ necessitates fixing the metric components, as well as their first, second, and third derivatives, thereby introducing more degrees of freedom compared to General Relativity. The emergence of these fourth-order terms in the metric can be avoided by considering the Gauss-Bonnet scalar [143]

$$\mathcal{G} = R^2 - 4R_{\alpha\beta}R^{\alpha\beta} + R_{\alpha\beta\gamma\delta}R^{\alpha\beta\gamma\delta}, \tag{1.45}$$

such that the action may be written as

$$S_{\mathcal{G}} = \int_{\mathcal{M}} d^4x\sqrt{-g}\mathcal{G} \tag{1.46}$$

There exists, however, a more general theory of modified gravities known as Lovelock Theories, which provides a generalization of the Gauss-Bonnet scalar [144]. Such theories are based on a general Lagrangian of the form

$$\mathcal{L}_L = \sqrt{-g}\sum_n \frac{1}{2^n}\alpha_n \delta^{\beta_1\beta_2\cdots\beta_{2n}}_{\gamma_1\gamma_2\cdots\gamma_{2n}} R^{\gamma_1\gamma_2\cdots}_{\beta_1\beta_2} R^{\gamma_{2n-1}\gamma_{2n}}_{\beta_{2n-1}\beta_{2n}} \tag{1.47}$$

where $\delta^{\beta_1\beta_2\cdots\beta_{2n}}_{\gamma_1\gamma_2\cdots\gamma_{2n}}$ is the generalized Kronecker delta of order $2n$, and α_n are constants.

Another interesting possibility, involves C^2 theories, where C denotes the Weyl tensor. These are termed Conformal Gravity theories, which possess the distinctive feature of being locally invariant and are candidates for the quantum formulation of gravity. The field equations in this conformal gravity were first published in [145], and their study is largely justified as a physically viable alternative to problems inherent in standard cosmology, particularly the dark matter hypothesis. Certain extensions of the Einstein-Hilbert action to models with higher order scalars are considered in [146–148].

Finally, a modification to General Relativity, known as $f(R)$ theories [96, 95, 97], is proposed, which consists of replacing the Einstein-Hilbert Lagrangian with an arbitrary function of the Ricci curvature scalar R.

Furthermore, it has been suggested that the observed accelerated expansion of the Universe might originate, among other possibilities, from corrections to the equations of motion of General Relativity. These corrections are generated by non-linear contributions of the curvature scalar R in the purely gravitational Lagrangian of $f(R)$ theories [97, 149–151]. In this context, relying on these contributions obviates the need for additional components, such as dark energy or a cosmological constant. Nonetheless, it has also been shown that solar system experiments appear to rule out those $f(R)$ theories capable of fitting the observed accelerated expansion. This constraint relies on the expansion in the weak-field limit of the $f(R)$ Lagrangian and the subsequent calculation of the Post-Newtonian coefficients [152–154]. Moreover, for the purposes of this thesis, $f(R)$ theories are considered unique among higher-order gravity theories as they are the only ones capable of circumvention the known Ostrogradsky instability [95].

In modified $f(R)$ gravity theories, we must distinguish between three distinct cases, which lead to different field equations. We possess two variational principles that can be applied to the Einstein-Hilbert action to derive the field equations: the usual variation with respect to the metric and the variation known as Palatini variation. In the latter, the metric and the connection are assumed to be independent variables, and the action is varied with respect to both, under the hypothesis that the contribution of the matter action is independent of the connection. Conversely, the choice of the variational principle is referred to in this case as the formalism; hence, they are denominated the metric formalism and the Palatini formalism, respectively. Both formalisms yield the same field equations for an action whose Lagrangian is linear in R; this equivalence does not hold for more general actions. The third version of the formalism for $f(R)$ theories is called the metric-affine formalism, which arises from utilizing the Palatini formalism while lifting the condition that the matter action contribution is independent of the connection. This final version is the most general possible within $f(R)$ theories, and it reduces to either the metric or Palatini formalisms under appropriate limits. In this thesis, we focus on the metric formalism, where the action is written as

$$S = S_{Met} + S_M\left(g_{\alpha\beta}, \phi\right), \tag{1.48}$$

with

$$S_{Met} = \frac{1}{2\kappa}\int_{\mathcal{M}} d^4x\sqrt{-g}f(R). \tag{1.49}$$

Here, $\kappa = 8\pi G$ and the variation is performed with respect to $g^{\mu\nu}$, and ϕ denotes the collection of all matter fields. In this context, $f(R)$ theories relax the condition that the Einstein-Hilbert action must be linear in the Ricci scalar R. This implies that the curvature term in the action is replaced by a function $f(R)$, which takes the general form

$$f(R) = \ldots + c_{-2}R^{-2} + c_{-1}R^{-1} - 2\Lambda + R + c_2R^2 + \ldots, \tag{1.50}$$

where the coefficients c_i determine the particular $f(R)$ gravity model. Varying the action with respect to the metric yields the following field equations (for a deeply detailed derivation see [155])

$$\frac{\delta S}{\delta g^{\mu\nu}} = f_R R_{\mu\nu} - \frac{1}{2}f(R)g_{\mu\nu} - \nabla_\mu\nabla_\nu f_R + g_{\mu\nu}\Box f_R = 2kT_{\mu\nu}, \tag{1.51}$$

where $f_R = \frac{df(R)}{dR}$,

$$\Box = \frac{1}{\sqrt{-g}}\partial_\mu \left(\sqrt{-g} g^{\mu\nu}\partial_\nu\right), \tag{1.52}$$

and the energy-momentum tensor $T_{\mu\nu}$ is defined by

$$T_{\mu\nu} = -\frac{2}{\sqrt{-g}}\frac{\delta S_M}{\delta g^{\mu\nu}}. \tag{1.53}$$

Expression (1.51) introduces fourth-order derivatives of the metric; hence, these theories are sometimes denoted as fourth-order gravity theories. It should be noted that in $f(R)$ theories, the energy-momentum tensor remains covariantly conserved, satisfying $\nabla_\mu T^{\mu\nu} = 0$ [156]. Let's remark that the espression (1.51) reduces to the standard Einstein field equations in the appropriate limit [154]. Additionally, $f(R)$ gravity possesses an inherent scalar degree of freedom, f_R, whose dynamics are determined by the trace of the generalized field equation, the so called scalaron [157, 158]. Consequently, these theories represent a significant generalization of General Relativity, particularly within the context of cosmological scenarios. For these reasons, we choose to investigate vacuum transitions incorporating this modification of the gravitational sector.

Chapter 2

Lorentzian vacuum transitions

In this section, we begin by discussing the general approach proposed in the references [50, 51], which employ the WKB approximation for the WDW equation. Specifically, the semiclassical decay rate contribution between a false vacuum and a true vacuum of a scalar field potential was computed and treated, based on it, the method introduced in the present section represents an extension, we will retrieved the semiclassical contribution in order to proceed with the higher order corrections of the WKB approximation. We adhere to the notation and conventions of these references. In this way, the WDW equation as show in Chapter 1, is obtained by performing a canonical quantization of the Hamiltonian constraint, specifically by substituting $\pi_M \to -i\hbar\frac{\delta}{\delta\Phi^M}$ in the last expression, leading to

$$\mathcal{H}\Psi(\Phi) = \left[-\frac{\hbar^2}{2}G^{MN}(\Phi)\frac{\delta}{\delta\Phi^M}\frac{\delta}{\delta\Phi^N} + \mathcal{V}[\Phi]\right]\Psi[\Phi] = 0, \tag{2.1}$$

up to ordering ambiguities[1]; where $\Psi[\Phi]$ is the wave functional in superspace. In order to obtain a semiclassical outcome and corrections of higher order, we take the general proposal of the WKB type

$$\Psi[\Phi] = \exp\left\{\frac{i}{\hbar}S[\Phi]\right\} \tag{2.2}$$

with the $\hbar$-expansion

$$S[\Phi] = S_0[\Phi] + \hbar S_1[\Phi] + \hbar^2 S_2[\Phi] + \mathcal{O}\left(\hbar^3\right). \tag{2.3}$$

Substituting this in the WDW equation (1.38) we obtain for the first three orders in $\hbar$

$$\frac{1}{2}G^{MN}\frac{\delta S_0}{\delta\Phi^M}\frac{\delta S_0}{\delta\Phi^N} + \mathcal{V}[\Phi] = 0, \tag{2.4}$$

$$2G^{MN}\frac{\delta S_0}{\delta\Phi^M}\frac{\delta S_1}{\delta\Phi^N} = iG^{MN}\frac{\delta^2}{\delta\Phi^M\delta\Phi^N}S_0, \tag{2.5}$$

$$2G^{MN}\frac{\delta S_0}{\delta\Phi^M}\frac{\delta S_2}{\delta\Phi^N} + G^{MN}\frac{\delta S_1}{\delta\Phi^m}\frac{\delta S_1}{\delta\Phi^N} = iG^{MN}\frac{\delta^2 S_1}{\delta\Phi^M\delta\Phi^N}. \tag{2.6}$$

Now, given a set of integral curves with parameter s defined on a particular slice on the space of fields, they are described by

$$C(s)\frac{d\Phi^M}{ds} = G^{MN}\frac{\delta S_0}{\delta\Phi^N}. \tag{2.7}$$

We can write down the classical contribution in the form

$$S_0\left[\Phi_s\right] = \int^{\Phi_s}\int_X \pi_M dx^M \tag{2.8}$$

[1]See Appendix A

which, by using Eqs. (2.4) and (2.7), it can be rewritten as

$$S_0\left[\Phi_s\right] = -2\int^s \frac{ds'}{C\left(s'\right)}\int_X \mathcal{V}\left[\Phi_{s'}\right]. \tag{2.9}$$

Manipulating equations (2.4) and (2.7) we find the following relation

$$G_{MN}\frac{d\Phi^M}{ds}\frac{d\Phi^N}{ds} = -\frac{2\mathcal{V}\left[\Phi_s\right]}{C^2(s)}, \tag{2.10}$$

where G_{MN} is the inverse of G^{MN}. We can see that Eqs. (2.7) and (2.10) form a system of $n+1$ equations for the $n+1$ variables: $\left(\frac{d\Phi^M}{ds}, C^2(s)\right)$ which in principle can be solved and then substituted back into the espression (2.9) to obtain the classical action and the superior order corrections. Let us assume that the fields Φ^M depend only on the time variable, then using (2.9), the variational derivative in (2.7) can be expressed in terms of a partial derivative of the function $\mathcal{V}[\Phi]$. Through this approach, the system can generally be solved, yielding solutions

$$\begin{aligned} C^2(s) &= -\frac{2\,\mathrm{Vol}^2(X)}{\mathcal{V}[\Phi]}G^{MN}\frac{\partial\mathcal{V}}{\partial\Phi^M}\frac{\partial\mathcal{V}}{\partial\Phi^N}, \\ \frac{d\Phi^M}{ds} &= \frac{\mathcal{V}[\Phi]}{\mathrm{Vol}(X)}\frac{G^{MN}\frac{\partial\mathcal{V}}{\partial\Phi^N}}{G^{LO}\frac{\partial\mathcal{V}}{\partial\Phi^L}\frac{\partial\mathcal{V}}{\partial\Phi^O}}, \end{aligned} \tag{2.11}$$

where, $\mathrm{Vol}(X)$ denotes the volume of the spatial slice, applicable under the assumption of field homogeneity, $\Phi^M = \Phi^M(s)$. It is pertinent to note that, in principle, $\mathrm{Vol}(X)$ may be infinite. However, by assuming a compactified spatial slice,we can forget about this term which, as we will demonstrate, will be a global general constant. From equation (2.11) we see that in general, we can obtain the following system of differential equations relating the various fields

$$\frac{d\Phi^M}{d\Phi^N} = \frac{G^{ML}\frac{\partial\mathcal{V}}{\partial\Phi^L}}{G^{NP}\frac{\partial\mathcal{V}}{\partial\Phi^P}}, \tag{2.12}$$

which is valid for every value of M and N such that $d\Phi^{M,N} \neq 0$. Therefore, the degrees of freedom are reduced in general and the classical action and the corrections will involve fewer fields in its computation. Now, considering the following order of the expansion, the first quantum correction, S_1, can be generally express as

$$\frac{dS_1}{ds} = \int_X \frac{d\Phi^M}{ds}\frac{\delta S_1}{\partial\Phi^M}, \tag{2.13}$$

such that, using (2.7) and (2.5), the above can be written as

$$S_1 = \frac{i}{2}\int_s\int_X \frac{ds}{C(s)}G^{MN}\frac{\delta^2 S_0}{\delta\Phi^M\delta\Phi^N}. \tag{2.14}$$

From (2.9), it stands out clearly that we can write

$$\frac{\delta S_0}{\delta\Phi^M} = -\frac{2\,\mathrm{Vol}(X)}{C(s)}\frac{\partial\mathcal{V}}{\partial\Phi^M}, \tag{2.15}$$

this can be used to obtain the system of equations for the general case. Then we can also write

$$\frac{\delta^2 S_0}{\delta\Phi^M\delta\Phi^N} = -\frac{2\,\mathrm{Vol}(X)}{C(s)}\frac{\partial^2\mathcal{V}}{\partial\Phi^M\partial\Phi^N} \tag{2.16}$$

wherewith is found for the action of the first correction

$$S_1 = -i\,\mathrm{Vol}^2(X)\int\frac{ds}{C^2(s)}G^{MN}\frac{\partial^2\mathcal{V}}{\partial\Phi^M\partial\Phi^N}. \tag{2.17}$$

Likewise, for the second order on $\hbar$, S_2, we have

$$\frac{dS_2}{ds} = \int_x \frac{d\Phi^M}{ds}\frac{\delta S_2}{\delta\Phi^M} = \int_x \frac{G^{MN}}{C(s)}\frac{\delta S_2}{\delta\Phi^M}\frac{\delta S_0}{\delta\Phi^N}, \tag{2.18}$$

wherein, we should employ (2.6) such that we have

$$G^{MN}\frac{\delta S_0}{\delta\Phi^M}\frac{\delta S_2}{\delta\Phi^N} = \frac{1}{2}G^{MN}\left(i\frac{\delta^2 S_1}{\delta\Phi^M\delta\Phi^N} - \frac{\delta S_1}{\delta\Phi^M}\frac{\delta S_1}{\delta\Phi^N}\right), \tag{2.19}$$

as well, substituting the above in (2.18), we get

$$\frac{dS_2}{ds} = \int_x \frac{1}{C(s)}\left(\frac{1}{2}\right)G^{MN}\left(i\frac{\delta^2 S_1}{\delta\Phi^M\delta\Phi^N} - \frac{\delta S_1}{\delta\Phi^M}\frac{\delta S_1}{\delta\Phi^N}\right), \tag{2.20}$$

$$S_2 = \frac{1}{2}\int_s\int_x \frac{ds}{C(s)}G^{MN}\left(i\frac{\delta^2 S_1}{\delta\Phi^M\delta\Phi^N} - \frac{\delta S_1}{\delta\Phi^M}\frac{\delta S_1}{\delta\Phi^N}\right). \tag{2.21}$$

If we take (2.14) and apply the functional derivative, we get

$$\frac{\delta S_1}{\partial\Phi^P} = -i\,\mathrm{Vol}^2(X)\frac{\partial}{\partial\bar{\Phi}^P}\left(\frac{G^{MN}}{C^2(s)}\frac{\partial^2\mathcal{V}}{\partial\Phi^M\partial\Phi^N}\right) \tag{2.22}$$

and

$$\begin{aligned}\frac{\delta S_1^2}{\delta\Phi^O\delta\Phi^P} = &-\frac{i\,\mathrm{Vol}^2(X)}{C^2(s)}\left(\frac{\partial^2 G^{MN}}{\partial\Phi^O\partial\Phi^P}\frac{\partial^2\mathcal{V}}{\partial\Phi^M\partial\Phi^N}\right.\\ &+\frac{\partial G^{MN}}{\partial\Phi^P}\frac{\partial^3\mathcal{V}}{\partial\Phi^O\partial\Phi^M\partial\Phi^N} + \frac{\partial G^{MN}}{\partial\Phi^O}\frac{\partial^3\mathcal{V}}{\partial\Phi^P\partial\Phi^M\partial\Phi^N}\\ &\left.+G^{MN}\frac{\partial^4\mathcal{V}}{\partial\Phi^O\partial\Phi^P\partial\Phi^M\partial\Phi^N}\right).\end{aligned} \tag{2.23}$$

So, finally, for the second correction, we get

$$\begin{aligned}S_2 =&\frac{1}{2}\int_s\int_X \frac{ds}{C(s)}G^{OP}\left[\frac{\mathrm{Vol}^2(X)}{C^2(s)}\left(\frac{\partial^2 G^{MN}}{\partial\Phi^O\partial\Phi^P}\frac{\partial^2\mathcal{V}}{\partial\Phi^M\partial\Phi^N} + \frac{\partial G^{MN}}{\partial\Phi^P}\frac{\partial^3\mathcal{V}}{\partial\bar{\Phi}^O\partial\Phi^M\partial\Phi^N}\right.\right.\\ &\left.+\frac{\partial G^{MN}}{\partial\Phi^O}\frac{\partial^3\mathcal{V}}{\partial\Phi^P\partial\Phi^M\partial\Phi^N} + G^{MN}\frac{\partial^4\mathcal{V}}{\partial\Phi^O\partial\Phi^P\partial\Phi^M\partial\Phi^N}\right)\\ &+\frac{\mathrm{Vol}^4(X)}{C^4(s)}\times\left(\frac{\partial G^{MN}}{\partial\Phi^O}\frac{\partial^2\mathcal{V}}{\partial\Phi^M\partial\Phi^N} + G^{MN}\frac{\partial^3\mathcal{V}}{\partial\Phi^O\partial\Phi^M\partial\Phi^N}\right)\times\\ &\left.\times\left(\frac{\partial G^{MN}}{\partial\Phi^P}\frac{\partial^2\mathcal{V}}{\partial\Phi^M\partial\Phi^N} + G^{MN}\frac{\partial^3\mathcal{V}}{\partial\Phi^P\partial\Phi^M\partial\Phi^N}\right)\right].\end{aligned} \tag{2.24}$$

or compactly

$$S_2 = \frac{1}{2}\int_s ds\frac{\mathrm{Vol}^3(X)}{C^3(s)}\nabla^2\left(\nabla^2\mathcal{V}\right) + \frac{1}{2}\int_s ds\frac{\mathrm{Vol}^5(X)}{C^5(s)}\left(\nabla\left(\nabla^2\mathcal{V}\right)\right)^2, \tag{2.25}$$

where

$$\nabla^2\mathcal{V} = G^{MN}\frac{\partial^2\mathcal{V}}{\partial\Phi^M\partial\Phi^N}, \quad (\nabla\mathcal{V})^2 = G^{MN}\frac{\partial\mathcal{V}}{\partial\Phi^M}\frac{\partial\mathcal{V}}{\partial\Phi^N}, \tag{2.26}$$

and we denoted in general

$$\nabla^M\mathcal{V} = G^{MN}\frac{\partial\mathcal{V}}{\partial\Phi^N}, \quad \nabla\mathcal{V}\cdot\nabla\mathcal{K} = G^{MN}\frac{\partial\mathcal{V}}{\partial\Phi^M}\frac{\partial\mathcal{K}}{\partial\Phi^N}. \tag{2.27}$$

In the context of this thesis, it will be deemed a wave functional corresponding to a path in field space in which the scalar field evolves from the false minimum to the true one, and one in which the system is kept at the false minimum during the path, so we can consider that the squared ratio of the absolute value of these wave functionals can be interpreted as the transition probability for the system to tunnel from the false to the true vacuum. Therefore, in the WKB approach considered here, the transition tunneling probability of going from the false vacuum at ϕ_A to the true vacuum at ϕ_B is the decay rate which is given by

$$P(A \to B) = \left| \frac{\Psi\left(\varphi_0^I, \phi_B; \varphi_m^I, \phi_A\right)}{\Psi\left(\varphi_0^I, \phi_A; \varphi_m^I, \phi_A\right)} \right|^2 = \left|e^{-\Gamma}\right|^2 = \exp[-2\,\mathrm{Re}(\Gamma)] \tag{2.28}$$

where we have denoted as φ^I the remaining fields on superspace apart from the scalar degree of freedom, $\Psi\left(\varphi_0^I, \phi_B, \varphi_m^I, \phi_A\right)$ is the wave functional corresponding to the path that starts in $\varphi^I(s=0) = \varphi_0^I$ with the scalar field ϕ_B and ends in $\varphi^I\left(s = s_M\right) = \varphi_m^I$ with the scalar field ϕ_A, and

$$\pm\Gamma = \frac{i}{\hbar}\left[S\left(\varphi_0^m, \phi_B; \varphi_M^m, \phi_A\right) - S\left(\varphi_0^m, \phi_A; \varphi_M^m, \phi_A\right)\right] \tag{2.29}$$

wherewith, using the expansion in the expression (2.3) up to second order, we end up with

$$\pm\Gamma = \Gamma_0 + \Gamma_1 + \Gamma_2, \tag{2.30}$$

where we have defined

$$\begin{cases} \Gamma_0 = \frac{i}{\hbar}[S_0\left(\varphi_0^m, \phi_B; \varphi_M^m, \phi_A\right) - S_0\left(\varphi_0^m, \phi_A; \varphi_M^m, \phi_A\right)], \\ \Gamma_1 = i\left[S_1\left(\varphi_0^m, \phi_B; \varphi_M^m, \phi_A\right) - S_1\left(\varphi_0^m, \phi_A; \varphi_M^m, \phi_A\right)\right], \\ \Gamma_2 = i\hbar\left[S_2\left(\varphi_0^m, \phi_B; \varphi_M^m, \phi_A\right) - S_2\left(\varphi_0^m, \phi_A; \varphi_M^m, \phi_A\right)\right]. \end{cases} \tag{2.31}$$

Γ_0 stands for the value that is calculated with the classical action, what would be referred to as the semiclassical contribution, Γ_1 is the first quantum correction, and Γ_2 is a second order correction; in terms of the expressions on (2.8), (2.14) and (2.25) these are written as

$$\begin{aligned} \Gamma_0 = -\frac{2\,\mathrm{Vol}(X) i}{\hbar} \Bigg\{ & \int_{s_0}^{\bar{s}-\delta s} \frac{ds}{C(s)} \mathcal{V}\bigg|_{\phi=\phi_B} - \int_{s_0}^{s-\delta s} \frac{ds}{C(s)} \mathcal{V}\bigg|_{\phi=\phi_A} \\ & + \int_{\bar{s}-\delta s}^{\bar{s}+\delta s} ds \left[\frac{\mathcal{V}}{C(s)} - \frac{\mathcal{V}}{C(s)}\bigg|_{\phi=\phi_A} \right] \Bigg\}, \end{aligned} \tag{2.32}$$

$$\begin{aligned} \Gamma_1 = \mathrm{Vol}^2(X) \Bigg[& \int_{s_0}^{\bar{s}-\delta s} \frac{ds}{C^2(s)} G^{MN} \frac{\partial^2 \mathcal{V}}{\partial \Phi^M \partial \Phi^N}\bigg|_{\phi=\phi_B} - \int_{s_0}^{\bar{s}-\delta s} \frac{ds}{C^2(s)} G^{MN} \frac{\partial^2 \mathcal{V}}{\partial \Phi^M \partial \Phi^N}\bigg|_{\phi=\phi_A} \\ & + \int_{\bar{s}-\delta s}^{\bar{s}+\delta s} ds \left(G^{MN} \frac{\partial^2 \mathcal{V}}{\partial \Phi^M \partial \Phi^N} \frac{1}{C^2(s)} - G^{MN} \frac{\partial^2 \mathcal{V}}{\partial \Phi^M \partial \Phi^N} \frac{1}{C^2(s)}\bigg|_{\phi=\phi_A} \right) \Bigg], \end{aligned} \tag{2.33}$$

$$\begin{aligned} \Gamma_2 = \frac{i\hbar}{2} \Bigg[& \int_{s_0}^{s-\delta s} ds \frac{\mathrm{Vol}^3(X)}{C^3(s)} \nabla^2\left(\nabla^2 \mathcal{V}\right)\bigg|_{\phi=\phi_B} + \int_{s_0}^{s-\delta s} ds \frac{\mathrm{Vol}^5(X)}{C^5(s)} \left(\nabla\left(\nabla^2 \mathcal{V}\right)\right)^2\bigg|_{\phi=\phi_B} \\ & - \int_{s_0}^{\bar{s}-\delta s} ds \frac{\mathrm{Vol}^3(x)}{C^3(s)} \nabla^2\left(\nabla^2 \mathcal{V}\right)\bigg|_{\phi=\phi_A} - \int_{s_0}^{\bar{s}-\delta s} ds \frac{\mathrm{Vol}^5(x)}{C^5(s)} \left(\nabla\left(\nabla^2 \mathcal{V}\right)\right)^2\bigg|_{\phi=\phi_A} \\ & + \int_{\bar{s}-\delta_s}^{\bar{s}+\delta_s} ds \frac{\mathrm{Vol}^3(X)}{C^3(s)} \left(\nabla^2\left(\nabla^2 \mathcal{V}\right) - \nabla^2\left(\nabla^2 \mathcal{V}\right)\big|_{\phi=\phi_A}\right) \\ & + \int_{\bar{s}-\delta_s}^{\bar{s}+\delta_s} ds \frac{\mathrm{Vol}^5(x)}{C^5(s)} \left(\left(\nabla\left(\nabla^2 \mathcal{V}\right)\right)^2 - \left(\nabla\left(\nabla^2 \mathcal{V}\right)\right)^2\Big|_{\phi=\phi_A}\right) \Bigg]. \end{aligned} \tag{2.34}$$

Although at this point we already have expressions for the decay rates, it is additionally possible to make a refinement to the previous expressions. First, considering that there are only quadratic terms of the canonical moments in the Hamiltonian restriction for the metrics considered in this thesis, we can rewrite the general solution in (2.11) as

$$C^2(s) = -\frac{2\,\mathrm{Vol}(X)}{\mathcal{V}}(\nabla\mathcal{V})^2, \quad \frac{d\Phi^M}{ds} = \frac{\mathcal{V}}{\mathrm{Vol}(X)}\frac{\nabla^M\mathcal{V}}{(\nabla\mathcal{V})^2}. \tag{2.35}$$

Second, in this thesis we will consider the matter content of the system to be only a scalar field canonically coupled to gravity with a potential that has a false and a true vacuum, whose action corresponds to General Relativity or $f(R)$ gravity action and the canonically coupled scalar field. We want to emphasize that, throughout this thesis, a specific functional form for the potential is not assumed. Instead, it is posited by construction that the potential possesses two distinct minima. Consequently, the derivatives of the potential evaluated at these critical points satisfy the standard conditions for local minima. This approach facilitates a more general analysis, requiring the specification of only the essential parameters.

We now specifically review for the Einstein-Hilbert action. Adopting natural units in which $c = 1$ and $8\pi G = 1$, the complete action under consideration is given by

$$S = \frac{1}{2}\int d^4x\sqrt{-g}R - \int d^4x\sqrt{-g}\left[\frac{1}{2}g^{\mu\nu}\partial_\mu\phi\partial_\nu\phi + V(\phi)\right], \tag{2.36}$$

allowing us to recast the function $\mathcal{V}$ as

$$\mathcal{V} = H\left(\varphi^I\right) + F\left(\varphi^I\right)V(\phi), \tag{2.37}$$

a estructure that will always appear due to the way in which the action of the scalar field is taken. The metric in the superspace will satisfy that $G^{I\phi} = 0$ if $I \neq \phi$. Again, this occurs because of the form of the scalar field action and always holds. Furthermore, we can assume that $G^{\phi\phi} = G^{\phi\phi}\left(\varphi^I\right)$ for the same reason, to wit, the dependence on the field comes in the function $\mathcal{V}$ through its potential. In conclusion, due to the fact that all fields in superspace can be related to the general solution, we can always write for constant scalar field regions $\mathcal{V} = \mathcal{V}\left(\Phi^i\right)$ for some fixed i that we choose. In this manner, the general solution can be cast as

$$C(s) = \pm i\,\mathrm{Vol}(X)\sqrt{\frac{2(\nabla\mathcal{V})^2}{\mathcal{V}}}, \quad ds = \frac{\mathrm{Vol}(X)(\nabla\mathcal{V})^2}{\mathcal{V}\nabla^i\mathcal{V}}d\Phi^i, \tag{2.38}$$

and be substituted in the general expressions in (2.32), (2.33) and (2.34). In addition, for the decay rate throughout all this thesis, in the terms where the potential is constant, we will apply the thin wall approximation, that is when $\delta s \to 0$. For the semiclassical contribution we have

$$\begin{aligned}\Gamma_0 = \mp\,&\frac{\sqrt{2}\,\mathrm{Vol}(X)}{\hbar}\left[\int_{\Phi_0^i}^{\bar{\Phi}^i}\left.\frac{\sqrt{\mathcal{V}(\nabla\mathcal{V})^2}}{\nabla^i\mathcal{V}}\right|_{\phi=\phi_B}d\Phi^i - \int_{\Phi_0^i}^{\bar{\Phi}^i}\left.\frac{\sqrt{\mathcal{V}(\nabla\mathcal{V})^2}}{\nabla^i\mathcal{V}}\right|_{\phi=\phi_A}d\Phi^i\right]\\ &+\frac{\mathrm{Vol}(X)}{\hbar}F\Big|_{\bar{\Phi}^i}T_0,\end{aligned} \tag{2.39}$$

where we have considered the contribution to the action originated from the path where the scalar field is not a constant as a tension term T. It was shown in [50, 51] that for the semiclassical solution these terms correspond to the bubble tension term appearing in the Euclidean approach. Thus, the tension term is defined as

$$\mathrm{Vol}(X)F|_{\bar{\Phi}^i}\,T_0 = -2\,\mathrm{Vol}(X)i\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{F}{C(s)}\left(V - V_A\right). \tag{2.40}$$

Following the same procedure, for the first correction we have

$$
\begin{aligned}
\Gamma_1 = &- \frac{\mathrm{Vol}(X)}{2}\left[\int_{\Phi_0^i}^{\bar{\Phi}^i} \frac{\nabla^2\mathcal{V}}{\nabla^i\mathcal{V}}\bigg|_{\phi=\phi_B} d\Phi^i - \int_{\Phi_0^i}^{\bar{\Phi}^i} \frac{\nabla^2\mathcal{V}}{\nabla^i\mathcal{V}}\bigg|_{\phi=\phi_A} d\Phi^i\right] \\
&+ \mathrm{Vol}(X)\left[\nabla_R^2 F\big|_{\bar{\Phi}^i} T_{1,1} + FG^{\phi\phi}\big|_{\bar{\Phi}^i} T_{1,2}\right],
\end{aligned} \tag{2.41}
$$

where $T_{1,1}$ and $T_{1,2}$ are tension parameters defined as in (2.40) for the previous case and $\nabla_R^2 F = G^{IJ}\frac{\partial^2}{\partial\varphi^I\partial\varphi^J}F$, i.e. restricted only to fields that are not the scalar field. Therefore we see that the global term of volume $\mathrm{Vol}(X)$ is generally holded in the first correction. Furthermore, to have only one tension term, one of the two terms must be zero or $\nabla_R^2 F = \zeta F G^{\phi\phi}$ needs to be true, where ζ is some constant. So, in general, we can have at most two tension terms. Finally, following the same procedure for the second correction, we find

$$
\begin{aligned}
\Gamma_2 = &\mp \frac{\mathrm{Vol}(X)\hbar}{4\sqrt{2}}\left[\int_{\Phi_0^i}^{\bar{\Phi}^i} \frac{\nabla^2\left(\nabla^2\mathcal{V}\right)}{\nabla^i\mathcal{V}}\sqrt{\frac{\mathcal{V}}{(\nabla\mathcal{V})^2}}\Bigg|_{\phi=\phi_B} d\Phi^i \right.\\
&\left. - \int_{\Phi_0^i}^{\bar{\Phi}^i} \frac{\nabla^2\left(\nabla^2\mathcal{V}\right)}{\nabla^i\mathcal{V}}\sqrt{\frac{\mathcal{V}}{(\nabla\mathcal{V})^2}}\Bigg|_{\phi=\phi_A} d\Phi^i\right] \\
&\pm \frac{\mathrm{Vol}(X)\hbar}{8\sqrt{2}}\left[\int_{\Phi_0^i}^{\bar{\Phi}^i} \frac{\left(\nabla\left(\nabla^2\mathcal{V}\right)\right)^2}{\nabla^i\mathcal{V}}\sqrt{\left(\frac{\mathcal{V}}{(\nabla\mathcal{V})^2}\right)^3}\Bigg|_{\phi=\phi_B} d\Phi^i \right.\\
&\left. - \int_{\Phi_0^i}^{\bar{\Phi}^i} \frac{\left(\nabla\left(\nabla^2\mathcal{V}\right)\right)^2}{\nabla^i\mathcal{V}}\sqrt{\left(\frac{\mathcal{V}}{(\nabla\mathcal{V})^2}\right)^3}\Bigg|_{\phi=\phi_A} d\Phi^i\right] \\
&+ \mathrm{Vol}(X)\hbar\left\{\nabla_R^2\left(\nabla_R^2 F\right)\big|_{\bar{\Phi}^i} T_{2,1} + \left[\left(\nabla_R^2 F\right)G^{\phi\phi} + \nabla_R^2\left(FG^{\phi\phi}\right)\right]\big|_{\bar{\Phi}^i} T_{2,2}\right. \\
&+ F\left(G^{\phi\phi}\right)^2\Big|_{\bar{\Phi}^i} T_{2,3} \\
&+ 2\nabla_R\left(\nabla_R^2 H\right)\cdot\nabla_R\left(\nabla_R^2 F\right)\big|_{\bar{\Phi}^i} T_{2,4} + \left[\nabla\left(\nabla_R^2 F\right)\right]^2\Big|_{\bar{\Phi}^i} T_{2,5} \\
&+ G^{\phi\phi}\left(\nabla_R^2 F\right)^2\Big|_{\bar{\Phi}^i} T_{2,6} \\
&+ 2F\left(G^{\phi\phi}\right)^2\nabla_R^2 F\Big|_{\bar{\Phi}^i} T_{2,7} + \nabla_R\left(\nabla_R^2 F\right)\cdot\nabla_R\left(FG^{\phi\phi}\right)\big|_{\bar{\Phi}^i} T_{2,8} \\
&+ 2\nabla_R\left(\nabla_R^2 H\right)\cdot\nabla_R\left(FG^{\phi\phi}\right)\big|_{\bar{\Phi}^i} T_{2,9} \\
&\left.+ \left[\nabla_R\left(FG^{\phi\phi}\right)\right]^2\Big|_{\bar{\Phi}^i} T_{2,10} + F^2\left(G^{\phi\phi}\right)^3\Big|_{\bar{\Phi}^i} T_{2,11}\right\},
\end{aligned} \tag{2.42}
$$

Where the terms $T_{2,i}$ with $i = 1, ..., 11$ are tension terms defined as above in (2.40). Therefore, in general we have the volume $\mathrm{Vol}(X)$ as a global term again. However, it is observed that there will be at most eleven tension terms that could be different. This quantity can only be reduced if some of them are zero or if they lead to the same form when considering a particular metric, as will be discussed in the following chapters.

On the other hand, as evidenced by the expressions for the tension terms associated with the quantum corrections, terms involving derivatives of the potential are inevitably generated. Consequently, in general, the definition of tension terms for any given order requires that the integrals across the domain wall be casted in the form

$$
\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\left[N\left(V(\phi), V^{(n)}(\phi)\right)O(\varphi^I)\right] ds, \tag{2.43}
$$

for specific functions $N\left(V(\phi), V^{(n)}(\phi)\right)$ and $O(\varphi^I)$, where $V^{(n)}$ denotes the nth derivative of the potential with respect to the scalar field. This condition is straightforwardly satisfied within the context of General Relativity. Nevertheless, as will be showed in Section 5, owing to the inherent structure of $f(R)$ theories, the separability condition implied by expression (2.43) may not be satisfied for arbitrary $f(R)$ models.

Chapter 3

Transition probabilities in 2+1 dimensions

Cosmology in three spacetime dimensions $(2+1)$ is an area of study motivated by the simplified nature of General Relativity in these dimensions, an approach that facilitates significant progress toward the general cosmological solution of Einstein's equations [162]. The theory exhibits unique characteristics, such as the absence of gravitational waves and the vanishing of the Weyl curvature, meaning spacetime geometry is entirely determined by the local matter distribution [163, 164]. To investigate the properties of these general relativistic cosmologies, covariant and first-order formalism techniques are employed. Detailed investigations address the search for general cosmological solutions, specifically for comoving and non-comoving dust matter, with or without a cosmological constant; the classification of their singular structures; the study of asymptotic behavior; and the identification of scalar field and pp-wave solutions [165, 166].

Furthermore, in recent years, there has been considerable interest in $(2+1)$ dimensional gravity. This interest stems, in part, from the fact that pure gravity can be exactly quantized in $(2+1)$ dimensions, thereby providing valuable insight into the more challenging problem of quantizing gravity in the physically realistic $3+1$ dimensional case. Unlike its higher-dimensional counterpart, $(2+1)$ dimensional gravity lacks local degrees of freedom, rendering it exactly solvable in many contexts while retaining rich global and topological structures. This makes it an ideal arena for probing foundational questions about quantum spacetime, tunneling processes, and the role of topology in gravitational physics.

The utility of $(2+1)$ gravity is particularly evident in studies of quantum tunneling and vacuum transitions. In [167] is demonstrated that a negative cosmological constant enables the nucleation of entire universes via quantum tunneling, providing a tractable model for cosmological birth scenarios that would be intractable in $(3+1)$ dimensions. Similarly, in [168] the nucleation of false vacuum bubbles is analyzed in this context, revealing how gravitational effects mediate quantum transitions between metastable vaca, a fundamental process for understanding the phase transitions of the early universe. Also, in [169] is establish that such tunneling events can induce topology change in spacetime itself, illustrating how quantum gravity may dynamically alter spatial geometry without singularities. These works collectively underscore $(2+1)$ gravity's capacity to model non-perturbative quantum gravity effects with analytical precision.

The framework's versatility extends to alternative formulations of gravity. It is shown in [170] that ISO(2,1) Chern-Simons theory; which is classically equivalent to $(2+1)$ Einstein gravity, naturally suit topology-changing transitions, bridging geometric and gauge theoretic perspectives on quantum gravity. This is reinforced by computing explicit transition amplitudes for topology change on a torus using Chern-Simons methods, highlighting the computational advantages of lower-dimensional models for path-integral approaches [171]. Meanwhile, the analysis of the

Wheeler-DeWitt equation in $(2+1)$ dimensions provided critical insights into the quantum constraints governing spacetime dynamics, demonstrating how reduced dimensionality clarifies the structure of quantum geometrodynamics [172]. Complementing these, a geometrodynamic approach to study quantum bubble evolution, further validating $(2+1)$ gravity as a consistent setting for semiclassical gravity calculations, is employed in [173]. These properties make $(2+1)$ dimensions a powerful theoretical laboratory for studying complex phenomena such as vacuum transitions, which are the subject of study in this thesis.

In this section, the formalism established in Section 2 is applied to General Relativity coupled to a scalar field in $(2+1)$ dimensions. The analysis is specifically conducted for flat and closed FLRW-type universes, as well as for Bianchi types I and III adapted to this dimensional framework.

3.1 Transitions for a Flat FLRW Metric

We commence this section by considering the Einstein-Hilbert action coupled to a scalar field in $2+1$ dimensions, given by

$$S = \frac{1}{2}\int d^3x\sqrt{-g}R - \int d^3x\sqrt{-g}\left[\frac{1}{2}g^{\mu\nu}\partial_\mu\phi\partial_\nu\phi + V(\phi)\right]. \tag{3.1}$$

The simplest cosmological model, corresponds to the flat FLRW metric in $2+1$ dimensions. This line element is explicitly expressed as

$$ds^2 = -N^2(t)dt^2 + a^2(t)\left(dx^2 + dy^2\right), \tag{3.2}$$

where $N(t)$ denotes the lapse function and $a(t)$ represents the scale factor. For this specific geometry, the corresponding Ricci scalar curvature is determined to be

$$R = \frac{2\dot{a}^2}{a^2N^2} - \frac{4\dot{a}\dot{N}}{aN^3} + \frac{4\ddot{a}}{aN^2}. \tag{3.3}$$

Substituting the explicit form of the metric (3.2) into the action (3.1), and subsequently performing an integration by parts to eliminate the second-order time derivatives (boundary terms), we obtain the gravitational contribution to the action as

$$\frac{1}{2}\int d^3x\sqrt{-g}R = \frac{\mathrm{Vol}(X)}{2}\int dt\left[\frac{2\dot{a}^2}{N} - \frac{4a\dot{a}\dot{N}}{N^2} + \frac{4a\ddot{a}}{N}\right] = -\frac{\mathrm{Vol}(X)}{2}\int \frac{2\dot{a}^2}{N}dt, \tag{3.4}$$

where $\mathrm{Vol}(X)$ denotes the volume of the spatial section, defined by the integration over the spatial coordinates

$$\mathrm{Vol}(X) = \iint dxdy. \tag{3.5}$$

Regarding the matter sector, assuming a homogeneous scalar field configuration $\phi(t)$ such that spatial gradients vanish, the matter action reduces to

$$\int d^3x\sqrt{-g}\left[\frac{1}{2}g^{\mu\nu}\partial_\mu\phi\partial_\nu\phi + V(\phi)\right] = \mathrm{Vol}(X)\int dt\left[-\frac{a^2\dot{\phi}^2}{2N} + Na^2V\right]. \tag{3.6}$$

Combining these results, the total Lagrangian for the system is determined to be

$$\mathcal{L} = -\frac{\dot{a}^2}{N} + \frac{a^2\dot{\phi}^2}{2N} - Na^2V. \tag{3.7}$$

The corresponding canonical momenta are derived via the standard definition $\pi_q = \frac{\partial\mathcal{L}}{\partial\dot{q}}$, yielding

$$\pi_N = 0, \quad \pi_a = -\frac{2\dot{a}}{N}, \quad \pi_\phi = \frac{\dot{\phi}a^2}{N}. \tag{3.8}$$

Performing the Legendre transformation leads to the Hamiltonian constraint

$$\mathcal{H} = \frac{N}{a^2}\left[\frac{\pi_\phi^2}{2} - \frac{a^2}{4}\pi_a^2 + a^4 V\right], \tag{3.9}$$

which exhibits a quadratic dependence on the momenta, analogous to the general Hamiltonian constraint (1.37) considered within the formalism developed in the preceding chapter. In (3.9), the term a^{-2} has been explicitly factored within the lapse function prefactor. This algebraic restructuring is strategically implemented to preserve a formal structural analogy with the formulation of the $3+1$ dimensional scenario [50, 51]. By casting the Hamiltonian in this specific guise, we seek to systematically investigate the impact of the specific algebraic factorization of the scale factor within the Hamiltonian constraint on the resulting transition probabilities. Given that the Hamiltonian constraint admits redefinitions via the lapse function which are classically equivalent but may imply distinct operator orderings upon quantization, it is crucial to determine whether such algebraic choices induce physical discrepancies in the semiclassical tunneling rates and quantum corrections. Specifically, this form reveals a diagonal minisuperspace metric with components

$$G^{aa} = -\frac{a^2}{2}, \quad G^{\phi\phi} = 1, \tag{3.10}$$

and the function

$$\mathcal{V} = a^4 V. \tag{3.11}$$

Following the general procedure, we obtain

$$\begin{aligned}\pm\Gamma_0 = &-\frac{2\,\mathrm{Vol}(X)i}{\hbar}\int_0^{\bar{s}-\delta s}\frac{a^4 V_B}{C(s)}ds + \frac{2\,\mathrm{Vol}(X)i}{\hbar}\int_0^{\bar{s}-\delta s}\frac{a^4 V_A}{C(s)}ds \\ &-\frac{2\,\mathrm{Vol}(X)i}{\hbar}\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{a^4}{C(s)}\left[V(\phi)-V_A\right]ds;\end{aligned} \tag{3.12}$$

to evaluate the first two integrals, we consider the general solution. Utilizing the general expression derived in equation (2.11), we determine the squared function $C^2(s)$ by substituting the specific minisuperspace metric components and the function $\mathcal{V}$. This yields the following expression

$$C^2(s) = \frac{-2\,\mathrm{Vol}^2(X)}{\mathcal{V}}\left[G^{aa}\left(\frac{\partial\mathcal{V}}{\partial a}\right)^2 + G^{\phi\phi}\left(\frac{\partial\mathcal{V}}{\partial\phi}\right)^2\right] = -\frac{2\,\mathrm{Vol}^2(X)}{V}\left(-8a^4V^2 + a^4 V^{(1)2}\right). \tag{3.13}$$

Correspondingly, the derivative of the scale factor a with respect to the parameter s is determined by

$$\frac{da}{ds} = \frac{\mathcal{V}}{\mathrm{Vol}(X)}\frac{G^{aa}\frac{\partial\mathcal{V}}{\partial a}}{\left[G^{aa}\left(\frac{\partial\mathcal{V}}{\partial a}\right)^2 + G^{\phi\phi}\left(\frac{\partial\mathcal{V}}{\partial\phi}\right)^2\right]} = \frac{-2aV^2}{\mathrm{Vol}(X)\left(V^{(1)2} - 8V^2\right)}. \tag{3.14}$$

Based on this relation, we proceed to evaluate the integrals over the regions characterized with constant field configuration, specifically corresponding to the local minima of the potential. In these regions, the first derivative of the potential vanishes, implying the condition $V^{(1)}_{A,B} = 0$, consequently, under these constraints, it is found that

$$\int \frac{\mathcal{V}}{C(s)}ds = \pm\int\sqrt{-\frac{\mathcal{V}}{2G^{aa}}}da = \pm\sqrt{V}\int a da. \tag{3.15}$$

Thus, we can write

$$\begin{aligned}\pm\Gamma_0 = &-\frac{2\,\mathrm{Vol}(X)i}{\hbar}(\pm\sqrt{V_B})\frac{a^2}{2}\bigg|_{a_0}^{\bar{a}} + \frac{2\,\mathrm{Vol}(X)i}{\hbar}(\pm\sqrt{V_A})\frac{a^2}{2}\bigg|_{a_0}^{\bar{a}} \\ &-\frac{2\,\mathrm{Vol}(X)i}{\hbar}\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{a^4}{C(s)}\left[V(\phi)-V_A\right]ds.\end{aligned} \tag{3.16}$$

Furthermore, since the function is well-behaved, we can choose for initial value of the factor scale, $a_0 = 0$ and define a tension term as

$$\mathrm{Vol}(X)\bar{a}^4 T_0 = -2\,\mathrm{Vol}(X) i \int_{\bar{s}-\delta s}^{\bar{s}+\delta s} \frac{a^4}{C(s)} \left[V(\phi) - V_A\right] ds. \tag{3.17}$$

Therefore, in the thin-wall limit $\delta s \to 0$, we obtain

$$\pm\Gamma_0 = \mp\frac{\mathrm{Vol}(X) i}{\hbar}(\sqrt{V_B} - \sqrt{V_A})\bar{a}^2 + \frac{\mathrm{Vol}(X)}{\hbar}\bar{a}^4 T_0, \tag{3.18}$$

which exhibits a form analogous to the $3+1$ dimensional case reported in [51]. We now proceed to calculate the first quantum correction. For this, it is necessary to evaluate the contraction of the second derivatives of $\mathcal{V}$ with the metric. Computing the partial derivatives with respect to the scale factor and the scalar field, this term is explicitly calculated as

$$\nabla^2\mathcal{V} = G^{MN}\frac{\partial^2\mathcal{V}}{\partial\Phi^M\partial\Phi^N} = G^{aa}\frac{\partial^2\mathcal{V}}{\partial a^2} + G^{\phi\phi}\frac{\partial^2\mathcal{V}}{\partial\phi^2} = a^4\left(V^{(2)} - 6V\right). \tag{3.19}$$

Finally, by substituting these intermediate results into the general expression (2.33), we arrive at the explicit form for the first quantum correction

$$\Gamma_1 = \frac{\mathrm{Vol}(X)}{4}\left(\frac{V_B^{(2)}}{V_B} - \frac{V_A^{(2)}}{V_A}\right)\ln(a)\Bigg|_{a_0}^{\bar{a}} - \mathrm{Vol}^2(X)\int_{\bar{s}-\delta s}^{\bar{s}+\delta s} a^4\frac{ds}{C^2(s)}\left(\tilde{V} - \tilde{V}_A\right), \tag{3.20}$$

where we have introduced $\tilde{V} = 6V - V^{(2)}$ where $\tilde{V}_A = \tilde{V}(V(\phi = \phi_A))$. We observe the presence of a logarithmic term in the derived expression. In order to consistently admit the boundary condition $a_0 = 0$ without introducing a divergence, it is necessary to impose a specific constraint on the coefficient accompanying this term. Consequently, we require that

$$\frac{V_B^{(2)}}{V_B} = \frac{V_A^{(2)}}{V_A}. \tag{3.21}$$

The satisfaction of this consistency condition assures the cancellation of the divergent terms, the remaining expression encapsulates the contribution arising solely from the transition region, thereby yielding a tension term. In this way we only kept a tension term, T_1, this tension is defined by the integral over the transition interval as follows

$$\mathrm{Vol}(X)\bar{a}^4 T_1 = -\,\mathrm{Vol}^2(X)\int_{\bar{s}-\delta s}^{\bar{s}+\delta s} a^4\frac{ds}{C^2(s)}\left(\tilde{V} - \tilde{V}_A\right). \tag{3.22}$$

So, we only have for the first quantum correction

$$\Gamma_1 = \mathrm{Vol}(X)\bar{a}^4 T_1, \tag{3.23}$$

It is evident that this expression exhibits the same functional dependence on the scale factor as the principal order tension term, T_0. Consequently, this quantum correction does not introduce new behavior; rather, it works as an additive contribution to the vacuum transition probability. Proceeding to the computation of the second quantum correction, the action term S_2 is evaluated as

$$S_2 = \frac{\mathrm{Vol}(X)}{2^{7/2}}\int\frac{da}{a^3}W, \tag{3.24}$$

where the function W, which encapsulates the higher-order derivatives of the potential, is defined by the expression

$$\begin{aligned} W =& \frac{-\left(36V - 12V^{(2)} + V^{(4)}\right)}{V^{1/2}\left(8V^2 - V^{(1)2}\right)^{1/2}} \\ &- \frac{V^{1/2}\left[-288V^2 + 36V^{(1)2} + 96VV^{(2)} - 8V^{(2)2} - 12V^{(1)}V^{(3)} + V^{(3)2}\right]}{2\left(8V^2 - V^{(1)2}\right)^{3/2}}. \end{aligned} \tag{3.25}$$

Consequently, utilizing this definition, the expression for the second correction to the transition probability, Γ_2, reduces to

$$\begin{aligned}\Gamma_2 = \mp \frac{i\hbar\,\mathrm{Vol}(X)}{2^{7/2}}\left[(W_B - W_A)\,\frac{1}{2a^2}\bigg|_{a_0}^{\bar{a}}\right] + \frac{i\hbar}{2}\int_{\bar{s}-\delta s}^{\bar{s}+\delta s} ds\frac{\mathrm{Vol}^3(X)}{C^3(s)}a^4\left(\bar{V} - \bar{V}_A\right)\\ + \frac{i\hbar}{2}\int_{\bar{s}-\delta s}^{\bar{s}+\delta s} ds\frac{\mathrm{Vol}^5(X)}{C^5(s)}a^8\left(\bar{\bar{V}} - \bar{\bar{V}}_A\right),\end{aligned} \tag{3.26}$$

where, for notational compactness, we have introduced the auxiliary definitions

$$\bar{V} = 36V - 12V^{(2)} + V^{(4)}, \tag{3.27}$$

and

$$\bar{\bar{V}} = -288V^2 + 36V^{(1)2} + 96VV^{(2)} - 8V^{(2)2} - 12V^{(1)}V^{(3)} + V^{(3)2}. \tag{3.28}$$

Analogous to the considerations employed for the first correction, in order to admit the choice of the initial boundary condition $a_0 = 0$ without introducing singular behavior, it is imperative to impose a constraint on the potential functions associated with the $1/a$ divergence. Specifically, this necessitates the equality $W_A = W_B$. Once this requirement is met, the divergent contributions at the boundaries cancel out, and the remaining expression reduces to two distinct tension terms, each with a unique functional dependence on the scale factor. Consequently, the final expression is given by

$$\Gamma_2 = \hbar\,\mathrm{Vol}(X)\bar{a}^4T_{2,1} + \hbar\,\mathrm{Vol}(X)\bar{a}^8T_{2,2}. \tag{3.29}$$

From these results, it is observed that by making an appropriate selection of the sign in (2.39), the transition probability, when including up to second order in quantum corrections, satisfies the condition $\lim_{\bar{a}\to 0} P(A \to B) = 1$. This behavior bears significant physical implications. Specifically, it demonstrates that the cumulative effect of the semiclassical contribution, alongside the first and second quantum corrections, simply causing the probability to decrease more rapidly with the corrections. Consequently, this result implies that the most probable initial size of the created universe corresponds to a zero volume.

Examining the analytic behavior of the derived contributions. Let us remark from (3.18) that the semiclassical contribution Γ_0 exhibits regular behavior across the entire domain of potential and scale factor values. While the expression may acquire an imaginary component for positive values of the potential minima, this is not a problem since we take only the real part always. Regarding the quantum corrections Γ_1 and Γ_2, we observe that they are characterized only by well-defined tension terms, a consequence of the procedure that eliminated the divergent contributions arising from the regions of constant field by imposing to specific constraints on the higher-order derivatives of the potential. We also want to note that for positive values of the potential will imply that that only tension terms predominate; for negative potentials, there will be only an additional contribution from the semiclassical term.

3.1.1 Hamiltonian of the form $H = N\mathcal{H}$

Now, in the spirit of exploring the formalism and the effect of factorization on the Hamiltonian constraint, we proceed in this section by considering the Hamiltonian initially presented in (3.9). However, we adopt an alternative factorization strategy, expressing the constraint as follows

$$H = N\left[\frac{-\pi_a^2}{4} + \frac{\pi_\phi^2}{2a^2} + a^2V\right]. \tag{3.30}$$

In this specific instance, the metric is characterized by the components

$$G^{aa} = -\frac{1}{2}, \quad G^{\phi\phi} = \frac{1}{a^2}, \tag{3.31}$$

and we will have th function

$$\mathcal{V} = a^2 V. \tag{3.32}$$

Adhering to the general procedure outlined previously, the semiclassical contribution is derived as

$$\begin{aligned}\pm\Gamma_0 = &-\frac{2\,\mathrm{Vol}(X)i}{\hbar}(\pm\sqrt{V_B})\frac{a^2}{2}\bigg|_{a_0}^{\bar{a}-\delta a} + \frac{2\,\mathrm{Vol}(X)i}{\hbar}(\pm\sqrt{V_A})\frac{a^2}{2}\bigg|_{a_0}^{\bar{a}-\delta a} \\ &-\frac{2\,\mathrm{Vol}(X)i}{\hbar}\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{a^2}{C(s)}\left[V(\phi)-V_A\right]ds.\end{aligned} \tag{3.33}$$

Given the behaviour of the function, we may again select the boundary condition $a_0 = 0$. In same fashion, we define a the tension term as in (3.17), such that in the thin-wall limit $\delta a \to 0$, we obtain

$$\pm\Gamma_0 = \mp\frac{\mathrm{Vol}(X)i}{\hbar}(\sqrt{V_B}-\sqrt{V_A})\bar{a}^2 + \frac{\mathrm{Vol}(X)}{\hbar}\bar{a}^2 T, \tag{3.34}$$

which exhibits an identical structure within the regions of constant field to that of the previous factorization. The sole distinction lies in the power of the scale factor a associated with the tension term, which now scales as $\bar{a}^2$ rather than a^4 found in the alternative ordering. Proceeding to the first quantum correction utilizing (2.33), we obtain

$$\Gamma_1 = \frac{\mathrm{Vol}(X)}{2}\left(\frac{V_B^{(2)}}{V_B}-\frac{V_A^{(2)}}{V_A}\right)\ln(a)\bigg|_{a_0}^{\bar{a}+\delta a} - \mathrm{Vol}^2(X)\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{ds}{C^2(s)}\left(\tilde{V}-\tilde{V}_A\right), \tag{3.35}$$

where we define $\tilde{V} = V - V^{(2)}$ with $\tilde{V}_A = \tilde{V}(V(\phi = \phi_A))$. It is evident that a logarithmic term reappears in the derived expression. To preclude the occurrence of indeterminacies and ensure a well-defined behavior, it is necessary to impose the consistency condition given by equation (3.21), analogous to the procedure employed in the preceding analysis. Consequently, upon satisfying this constraint and defining the corresponding tension term, the expression for the first quantum correction simplifies significantly, reducing to

$$\Gamma_1 = \mathrm{Vol}(X)T_1. \tag{3.36}$$

In contrast to the previous factorization case, where the correction retained a dependence on the scale factor, this contribution manifests as a constant value, dependent only on the spatial volume and the tension T_1. This implies that the transition probability limit as $a \to 0$ yields a finite value strictly less than unity, provided that an appropriate choice of signs is maintained. Regarding the second correction, we have

$$\begin{aligned}\Gamma_2 = &\mp\frac{i\hbar\,\mathrm{Vol}(X)}{2^{5/2}}\left[(W_B-W_A)\frac{1}{2a^2}\bigg|_{a_0}^{\bar{a}-\delta a}\right] + \frac{i\hbar}{2}\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}ds\frac{\mathrm{Vol}^3(X)}{C^3(s)}\frac{1}{a^2}\left(\bar{V}-\bar{V}_A\right) \\ &+\frac{i\hbar}{2}\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}ds\frac{\mathrm{Vol}^5(X)}{C^5(s)}\frac{1}{a^2}\left(\bar{\bar{V}}-\bar{\bar{V}}_A\right),\end{aligned} \tag{3.37}$$

with the auxiliary definitions

$$W = \frac{-V^{(4)}+V^{(2)}}{V^{1/2}\left(2V^2-V^{(1)2}\right)^{1/2}} - \frac{V^{1/2}\left(-V^{(1)}+V^{(3)}\right)^2}{2\left(2V^2-V^{(1)2}\right)^{3/2}}, \tag{3.38}$$

$$\bar{V} = -V^{(2)} + V^{(4)}, \tag{3.39}$$

and

$$\bar{\bar{V}} = \left(V^{(3)}-V^{(1)}\right)^2. \tag{3.40}$$

As observed, the second quantum correction manifests a term that scales as a^{-2} within the region of constant scalar field. Consequently, to rigorously admit the initial value $a_0 = 0$ without encountering a singularity, it is necessary to impose the consistency constraint $W_A = W_B$. This requirement ensures the cancellation of the divergent contributions at the origin, thereby rendering the transition probability well-defined. With respect to the two remaining terms, it is observed that although they arise from distinct integral contributions within the eleven terms shown in (2.42), they exhibit an identical functional dependence on the scale factor. This structural similarity allows for their consideration into a single effective tension parameter, denoted as T_2. Consequently, the final expression for the second quantum correction simplifies to

$$\Gamma_2 = \frac{\mathrm{Vol}(X)\hbar}{\bar{a}^2} T_2. \tag{3.41}$$

It is pertinent to note that, with the appropriate selection of signs, the transition probability satisfies the limit $\lim_{\bar{a}\to 0} P(A \to B) = 0$. This behavior has profound physical implications; specifically, it indicates that the inclusion of the second-order quantum correction suppresses the probability of transition at a vanishing scale factor. Consequently, the most probable initial configuration of the universe corresponds to a finite, non-zero value of the scale factor. In this manner, the quantum correction terms provide a mechanism that avoids the classical spatial singularity.

Having examined both factorization schemes, in this first test using the flat FLRW metric, we observe that at the lowest order of the WKB expansion, there is no substantial deviation in the functional form of the semiclassical amplitude Γ_0, with the exception of the power of the scale factor associated with the tension term. Specifically, the explicit factorization of $1/a^2$ shifts this exponent from 2 to 4. Consequently, for scale factor values $\bar{a} < 1$, this modification results in a diminished impact, whereas for values $\bar{a} > 1$, it induces a more rapid decay of the transition probability. The true significance of these distinct factorizations becomes apparent upon the inclusion of quantum corrections. Notably, we observe that in the absence of this specific factorization, the initial singularity becomes accessible when the analysis is extended to include the second quantum correction. Motivated by this observation, and leveraging the tractability of the $(2+1)$ dimensional framework, we proceed to explore the specific effects of these factorizations on the transition probabilities for the remaining metrics considered within this thesis.

3.2 Transitions for a Closed FLRW Metric

Now, in this section, we consider the case of positive spatial curvature. In the familiar context of $(3+1)$ dimensions, the closed FLRW metric is expressed using hyperspherical coordinates. For our specific purpose in $(2+1)$ dimensions, the spatial section corresponds to a 2-sphere (S^2). Consequently, the metric can be written as

$$ds^2 = -N^2(t)dt^2 + a^2(t)\left(dr^2 + \sin^2 r d\theta^2\right), \tag{3.42}$$

where the radial coordinate $r \in [0, \pi]$ and the angular coordinate $\theta \in [0, 2\pi]$. Following the established procedure and substituting this metric into the action (3.1), the resulting Lagrangian is given by

$$\mathcal{L} = N - \frac{\dot{a}^2}{N} + \frac{a^2\dot{\phi}^2}{2N} - a^2 NV. \tag{3.43}$$

It is observed that the canonical momenta derived from this Lagrangian are identical to those obtained for the flat FLRW metric. However, the resulting Hamiltonian constraint acquires an additional term due to the spatial curvature

$$\mathcal{H} = N\left[\frac{\pi_\phi^2}{2a^2} - \frac{\pi_a^2}{4} + a^2 V - 1\right]. \tag{3.44}$$

We observe that the structure of the constraint remains consistent with the previous cases (modulo a factor of a^2), but with the effective potential function modified to $\mathcal{V} = a^2 V - 1$. Proceeding with the calculation of the spatial volume for this geometry, we have

$$\mathrm{Vol}(X) = \int_{\theta=0}^{2\pi} \int_{r=0}^{\pi} \sin r dr d\theta = 4\pi. \tag{3.45}$$

Therefore, applying the formalism, the transition probability is expressed as

$$\pm\Gamma = -\frac{8\pi i}{\hbar} \int_0^{\bar{s}-\delta s} \frac{a^2 V_B - 1}{C(s)} ds + \frac{8\pi i}{\hbar} \int_0^{\bar{s}-\delta s} \frac{a^2 V_A - 1}{C(s)} ds - \frac{8\pi i}{\hbar} \int_{\bar{s}-\delta s}^{\bar{s}+\delta s} \frac{a^2}{C(s)} \left[V(\phi) - V_A\right] ds. \tag{3.46}$$

Once again, as in the Flat FLRW case, we define the tension term T_0 via the final integral over the wall width

$$4\pi \bar{a}^2 T_0 = -4\pi i \int_{\bar{s}-\delta s}^{\bar{s}+\delta s} \frac{a^2}{C(s)} \left[V(\phi) - V_A\right] ds. \tag{3.47}$$

For the first two integrals, the general solution is obtained by transforming the integration variable to the scale factor a. This yields

$$\frac{8\pi i}{\hbar} \int \frac{\mathcal{V}}{C(s)} ds = \pm \frac{8\pi i}{\hbar} \int \sqrt{-\frac{\mathcal{V}}{2G^{aa}}} da = \pm \frac{8\pi i}{\hbar} \int \sqrt{a^2 V - 1} da = \mp \frac{8\pi}{\hbar} \int \sqrt{1 - a^2 V} da. \tag{3.48}$$

Furthermore, in the thin-wall limit, the expression simplifies to

$$\pm\Gamma_0 = \pm \frac{8\pi}{\hbar} \left[\int_{a_0}^{\bar{a}} \sqrt{1 - a^2 V_B} da - \int_{a_0}^{\bar{a}} \sqrt{1 - a^2 V_A} da \right] + 4\pi \bar{a}^2 T_0. \tag{3.49}$$

To evaluate these integrals explicitly, we utilize the standard integration result

$$\int \sqrt{1 - Cx^2} dx = \frac{x}{2} \sqrt{1 - Cx^2} + \frac{1}{\sqrt{C}} \arctan\left(\frac{\sqrt{C} x}{\sqrt{1 - Cx^2} - 1} \right). \tag{3.50}$$

Applying this to our result, it is found that the lower limit $a_0 = 0$ can be chosen consistently, as its contribution cancels out between the two terms. This leaves the final semiclassical transition probability as

$$\begin{aligned} \pm\Gamma_0 = \pm \frac{8\pi}{\hbar} &\left[\frac{\bar{a}^2}{2} \left(\sqrt{1 - \bar{a}^2 V_B} - \sqrt{1 - \bar{a}^2 V_A} \right) + \frac{1}{\sqrt{V_B}} \arctan\left(\frac{\sqrt{V_B} \bar{a}}{\sqrt{1 - V_B \bar{a}^2} - 1} \right) \right. \\ &\left. - \frac{1}{\sqrt{V_A}} \arctan\left(\frac{\sqrt{V_A} \bar{a}}{\sqrt{1 - V_A \bar{a}^2} - 1} \right) \right] + 4\pi \bar{a}^2 T_0. \end{aligned} \tag{3.51}$$

This result exhibits a significantly distinct functional form compared to the $3+1$ dimensional case [50, 51], reflecting the topological and geometric differences inherent to the dimensionality of the spacetime. Continuing with the obtention of the first quantum correction, we retain the general structural form of expression (2.33). Consequently, the evaluation of the integral, evaluated at regions of constant scalar field, yields

$$\mathrm{Vol}^2(X) \int \frac{ds}{C^2(s)} \nabla^2 \mathcal{V} \Big|_{\phi=\phi_{A,B}} = -2\pi \left(\frac{V^{(2)}}{V} - 1 \right) \int \frac{da}{a} = -2\pi \left(\frac{V^{(2)}}{V} - 1 \right) \ln a. \tag{3.52}$$

Furthermore, the contribution arising from the wall term is expressed as

$$\mathrm{Vol}^2(X) \int_{\bar{s}-\delta s}^{\bar{s}+\delta s} ds \left(\frac{\nabla^2 \mathcal{V}}{C^2(s)} - \frac{\nabla^2 \mathcal{V}}{C^2(s)} \Big|_{\phi=\phi_A} \right) = -16\pi^2 \int_{\bar{s}-\delta s}^{\bar{s}+\delta s} \frac{ds}{C^2(s)} \left[\tilde{V} - \tilde{V}_A \right]. \tag{3.53}$$

Observing that this expression preserves the general functional form established previously, we define the tension parameter, T_1, as follows

$$4\pi T_1 = -8\pi \int_{\bar{s}-\delta s}^{\bar{s}+\delta s} \frac{ds}{C^2(s)} \left[\tilde{V} - \tilde{V}_A\right]. \tag{3.54}$$

Consequently, the explicit form of the first quantum correction is given by

$$\Gamma_1 = 2\pi \left(\frac{V_A^{(2)}}{V_A} - \frac{V_B^{(2)}}{V_B} \right) \ln a \Bigg|_{a_0}^{\bar{a}} + 8\pi^2 T_1. \tag{3.55}$$

It is worth noting the same singularity as for the flat FLRW case. So, as well, if we attempt to impose the boundary condition $a_0 = 0$ in the general case, the logarithmic term diverges, causing the transition probability to vanish. This would seemingly necessitate the choice $a_0 \neq 0$. The only mathematical recourse to maintain the choice $a_0 = 0$ is to require that the potentials at the minima satisfy the constraint in (3.21). This condition can only be satisfied if the potentials share the same sign. Under this constraint, the logarithmic divergence is eliminated, and the quantum correction reduces to a constant value. Incorporating this consideration and utilizing the semiclassical result derived previously, the total transition probability is finally obtained as

$$\begin{aligned}\pm\Gamma = \pm\frac{8\pi}{\hbar} \Bigg[&\frac{\bar{a}^2}{2} \left(\sqrt{1-\bar{a}^2 V_B} - \sqrt{1-\bar{a}^2 V_A} \right) + \frac{1}{\sqrt{V_B}} \arctan\left(\frac{\sqrt{V_B}\bar{a}}{\sqrt{1-V_B\bar{a}^2}-1} \right) \\ &- \frac{1}{\sqrt{V_A}} \arctan\left(\frac{\sqrt{V_A}\bar{a}}{\sqrt{1-V_A\bar{a}^2}-1} \right) \Bigg] + \frac{4\pi\bar{a}^2}{\hbar} T_0 + 8\pi^2 T_1.\end{aligned} \tag{3.56}$$

We observe that in the limit $\bar{a} \to 0$, the expression reduces to $\Gamma = 8\pi^2 T_1$. This implies the condition $\pm T_1 \geq 0$, indicating that the initial value of the probability amplitude is modified by the quantum effects, just as the flat FLRW case. While the general functional behavior remains qualitatively similar to the semiclassical term, the probability originates from a value strictly less than the unity, rather than unity. Regarding the second quantum correction, we have

$$\begin{aligned}\Gamma_2 = \frac{i\hbar}{2} \Bigg\{ &-\frac{\mathrm{Vol}(X)}{6\sqrt{2}} \frac{\left(a^2 V_B - 1\right)^{\frac{3}{2}}}{a^3} \bar{V}_B + \frac{\mathrm{Vol}(X)}{10\sqrt{2}} \frac{\left(a^2 V_B - 1\right)^{\frac{5}{2}}}{a^5} \bar{\bar{V}}_B \\ &- \left[-\frac{\mathrm{Vol}(X)}{6\sqrt{2}} \frac{\left(a^2 V_A - 1\right)^{\frac{3}{2}}}{a^3} \bar{V}_A + \frac{\mathrm{Vol}(X)}{10\sqrt{2}} \frac{\left(a^2 V_A - 1\right)^{\frac{5}{2}}}{a^5} \bar{\bar{V}}_A \right] \Bigg\} \Bigg|_{a_0}^{\bar{a}} \\ &+ \frac{i\hbar}{2} \mathrm{Vol}^3(X) \int_{\bar{s}-\delta s}^{\bar{s}+\delta s} \frac{ds}{C^3(s)} \left(\frac{1}{a^2} \right) \left[\left(V^{(4)} - V^{(2)} \right) - \left(V_A^{(4)} - V_A^{(2)} \right) \right] \\ &+ \frac{i\hbar}{2} \mathrm{Vol}^5(X) \int_{\bar{s}-\delta s}^{\bar{s}+\delta s} \frac{ds}{C^5(s)} \left(\frac{1}{a^2} \right) \left[\left(V^{(1)} - V^{(3)} \right)^2 - \left(V_A^{(1)} - V_A^{(3)} \right)^2 \right],\end{aligned} \tag{3.57}$$

where, for the sake of notational brevity, we have introduced the auxiliary functions $\bar{V}$ and $\bar{\bar{V}}$, which encode the dependence on the higher order derivatives of the potential. These are defined explicitly as

$$\bar{V} = \frac{V^{(2)} - V^{(4)}}{V\left(2V^2 - V^{(1)2}\right)^{1/2}}, \tag{3.58}$$

and

$$\bar{\bar{V}} = \frac{\left(V^{(1)} - V^{(3)}\right)^2}{2V\left(2V^2 - V^{(1)2}\right)^{3/2}}. \tag{3.59}$$

In this manner, analogous to the flat case, it is observed that the terms associated with the wall can be grouped into a single effective tension term, as they exhibit an identical functional dependence on the scale factor. So we are left with

$$\begin{aligned}\Gamma_2 = \frac{i\hbar}{2}\Bigg\{ & -\frac{\mathrm{Vol}(X)}{6\sqrt{2}}\frac{\left(a^2V_B-1\right)^{\frac{3}{2}}}{a^3}\bar{V}_B+\frac{\mathrm{Vol}(X)}{10\sqrt{2}}\frac{\left(a^2V_B-1\right)^{\frac{5}{2}}}{a^5}\bar{\bar{V}}_B \\ & -\left[-\frac{\mathrm{Vol}(X)}{6\sqrt{2}}\frac{\left(a^2V_A-1\right)^{\frac{3}{2}}}{a^3}\bar{V}_A+\frac{\mathrm{Vol}(X)}{10\sqrt{2}}\frac{\left(a^2V_A-1\right)^{\frac{5}{2}}}{a^5}\bar{\bar{V}}_A\right]\Bigg\}\Bigg|_{a_0}^{\bar{a}} \\ & +\frac{\mathrm{Vol}(X)\hbar}{\bar{a}^2}T_2.\end{aligned} \tag{3.60}$$

For this metric, it is observed that the inclusion of the second quantum correction precludes the direct selection of the condition $a_0 = 0$, in contrast to the flat case. Nevertheless, the tension term remains identical in both instances. Furthermore, it is noteworthy that for scale factor values less than unity, the contributions arising from the regions of constant field remain real valued for both positive and negative potentials. Consequently, although access to the initial singularity is strictly prohibited in this regime, an initial value in its immediate vicinity may be considered, preserving the same behavior as in the flat case.

Given the structural similarity of the metrics, the explicit application of the alternative factorization is deemed unnecessary for this specific case, as the resulting physical behavior is expected to be analogous. However, the implications of different factorization scheme will be rigorously examined when addressing scenarios with anisotropy.

3.3 Transitions for a Bianchi Type I Metric

In this section, we examine the Bianchi Type I model, which constitutes the simplest anisotropic cosmological scenario. To this end, we reconsider the action defined in (3.1), incorporating the anisotropic Bianchi Type I metric in $(2+1)$ dimensions characterized by the line element

$$ds^2 = -N^2dt^2 + A(t)^2dx^2 + B(t)^2dy^2. \tag{3.61}$$

For this geometry, the square root of the determinant of the metric is given by

$$\sqrt{-g} = NAB, \tag{3.62}$$

and the Ricci scalar is calculated as

$$R = \frac{2[N(\dot{A}\dot{B} + B\ddot{A} + A\ddot{B}) - N(\dot{A}B + A\dot{B})]}{ABN^3}. \tag{3.63}$$

Consequently, the action can be rewritten in terms of the scale factors $A(t)$ and $B(t)$ as

$$S = \mathrm{Vol}(X)\int dt\left[-\frac{\dot{A}\dot{B}}{N} + \frac{AB\dot{\phi}^2}{2N} - NABV\right], \tag{3.64}$$

where $\mathrm{Vol}(X)$ is defined as in (3.5). From this expression, we identify the Lagrangian of the system

$$\mathcal{L} = -\frac{\dot{A}\dot{B}}{N} + \frac{AB\dot{\phi}^2}{2N} - NABV(\phi). \tag{3.65}$$

The corresponding canonical momenta are derived as

$$\pi_N = 0, \quad \pi_A = -\frac{\dot{B}}{N}, \quad \pi_B = -\frac{\dot{A}}{N}, \quad \pi_\phi = \frac{AB\dot{\phi}}{N}. \tag{3.66}$$

These momenta allow us to construct the Hamiltonian constraint

$$\mathcal{H} = \frac{N}{AB}\left[-\pi_A\pi_B AB + \frac{\pi_\phi^2}{2} + A^2B^2V(\phi)\right]. \tag{3.67}$$

We observe that this Hamiltonian possesses the same structural form as the general constraint (1.37). In this context, the non-zero components of the metric G^{MN} are identified as

$$G^{MN} = \begin{pmatrix} 0 & -AB & 0 \\ -AB & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{3.68}$$

and the function is given by $\mathcal{V} = A^2B^2V(\phi)$. Proceeding with the calculation, we define the potential values at the critical points. Following the general procedure, the semiclassical transition probability is expressed as

$$\begin{aligned}\pm\Gamma_0 = \frac{i}{\hbar}(-2\,\mathrm{Vol}(X))\Bigg\{&\int_0^{\bar{s}-\delta s}\frac{ds}{C(s)}A^2B^2V_B - \int_0^{\bar{s}-\delta s}\frac{ds}{C(s)}A^2B^2V_A \\ &+\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{ds}{C(s)}A^2B^2\left[V(\phi)-V_A\right]\Bigg\},\end{aligned} \tag{3.69}$$

where the function $C(s)$ function $C^2(s) = 16\,\mathrm{Vol}^2(X)A^2B^2V$. The derivatives of the scale factors with respect to the parameter s are governed by the system

$$\begin{cases} \frac{dA}{ds} = \frac{A}{4\,\mathrm{Vol}(X)} \\ \frac{dB}{ds} = \frac{B}{4\,\mathrm{Vol}(X)} \end{cases} \tag{3.70}$$

Based on the previous expression, it is evident that the scale factors are proportional, satisfying $A = b_0B$, where b_0 is a constant of integration. Assuming regular behavior, we set the lower integration limit to $A_0 = 0$. In the thin-wall limit the final expression for the transition probability is obtained as

$$\begin{aligned}\pm\Gamma_0 = &\mp\frac{\mathrm{Vol}(X)i}{\hbar}\left(b_{0B}\sqrt{V_B} - b_{0A}\sqrt{V_A}\right)\bar{A}^2 \\ &+\frac{\mathrm{Vol}(X)A^2B^2T_0}{\hbar},\end{aligned} \tag{3.71}$$

where the tension term, representing the contribution from the domain wall, is defined by

$$\mathrm{Vol}(X)A^2B^2T_0 = -2\,\mathrm{Vol}(X)i\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{ds}{C(s)}A^2B^2\left[V-V_A\right]. \tag{3.72}$$

Thus, to evaluate the first quantum correction, it is necessary to compute the contraction of the second derivatives of the function $\mathcal{V}$ with the superspace metric. This calculation proceeds as follows

$$\begin{aligned}\nabla^2\mathcal{V} = G^{MN}\frac{\partial^2\mathcal{V}}{\partial\Phi^M\partial\Phi^N} &= 2G^{AB}\frac{\partial^2\mathcal{V}}{\partial A\partial B} + G^{\phi\phi}\frac{\partial^2\mathcal{V}}{\partial\phi^2} \\ &= \left(-8A^2B^2V + A^2B^2V^{(2)}\right).\end{aligned} \tag{3.73}$$

Subsequently, substituting these results into the general expression given in (2.33), we obtain the explicit form for the first correction

$$\Gamma_1 = \frac{\mathrm{Vol}(X)}{4}\left(\frac{V_B^{(2)}}{V_B} - \frac{V_A^{(2)}}{V_A}\right)\ln(A)\Bigg|_{A_0}^{\bar{A}} - \mathrm{Vol}^2(X)\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{ds}{C^2(s)}A^2B^2\left(\tilde{V}-\tilde{V}_A\right), \tag{3.74}$$

where we have defined $\tilde{V} = 8V - V^{(2)}$ with $\tilde{V}_A = \tilde{V}(V(\phi = \phi_A))$. Finally, regarding the second quantum correction, the evaluation of the corresponding terms yields the following expression for Γ_2. This result incorporates the boundary contributions associated with the scale factor limits, as well as the integral terms arising from the potential modifications within the transition region

$$\begin{aligned}\Gamma_2 = &\frac{i\hbar\,\mathrm{Vol}(X)}{2^{9/2}}\left(W_B - W_A\right)\frac{1}{A^2}\bigg|_{A_0}^{\bar{A}} \\ &+ \frac{i\hbar\,\mathrm{Vol}^3(X)}{2}\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{ds}{C^3(s)}A^2B^2\left[\bar{V} - \bar{V}_A\right] \\ &+ \frac{i\hbar\,\mathrm{Vol}^5(X)}{2}\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{ds}{C^5(s)}A^4B^4\left[\bar{\bar{V}} - \bar{\bar{V}}_A\right],\end{aligned} \tag{3.75}$$

where the auxiliary functions W, $\bar{V}$, and $\bar{\bar{V}}$, which encapsulate the dependence on the higher-order derivatives of the potential, are explicitly defined as follows

$$\begin{aligned}W = &-\frac{\left(64V - 16V^{(2)} + V^{(4)}\right)}{V^{1/2}\left(8V^2 - V^{(1)2}\right)^{1/2}} \\ &- \frac{V^{1/2}\left(-512V^2 + 64V^{(1)2} + 128VV^{(2)} - 8V^{(2)2} - 16V^{(1)}V^{(3)} + V^{(3)2}\right)}{2\left(8V^2 - V^{(1)2}\right)^{3/2}},\end{aligned} \tag{3.76}$$

$$\bar{V} = 64V - 16V^{(2)} + V^{(4)}, \tag{3.77}$$

and

$$\bar{\bar{V}} = -512V^2 + 64V^{(1)2} + 128VV^{(2)} - 8V^{(2)2} - 16V^{(1)}V^{(3)} + V^{(3)2}. \tag{3.78}$$

We observe that, given the relationship between the metric scale factors $A = b_0 B$, this result is identical to that obtained for the flat case. Consequently, no further simplification is presented.

3.3.1 Hamiltonian of the form $H = N\mathcal{H}$

On the other hand, to ensure that the results corresponding to the flat case are identically recovered, we consider the alternative ordering for the Hamiltonian,

$$H = N\left[-\pi_A\pi_B + \frac{\pi_\phi^2}{2AB} + ABV(\phi)\right]. \tag{3.79}$$

From this expression, we identify the components of the metric as

$$G^{MN} = \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & \frac{1}{AB} \end{pmatrix}, \tag{3.80}$$

and the function

$$\mathcal{V} = ABV. \tag{3.81}$$

Proceeding with the established procedure, we obtain the squared constraint function

$$C^2(s) = 4\,\mathrm{Vol}^2(X)V. \tag{3.82}$$

The relationship between the scale factors A and B remains preserved,

$$A = b_0 B, \tag{3.83}$$

such that the semiclassical transition probability is given by

$$\begin{aligned}\pm\Gamma_0 = &\mp \frac{\mathrm{Vol}(X)i}{\hbar}\left(b_{0B}\sqrt{V_B} - b_{0A}\sqrt{V_A}\right)\bar{A}^2 \\ &+ \frac{\mathrm{Vol}(X)ABT_0}{\hbar},\end{aligned} \tag{3.84}$$

with the tension term defined as

$$\mathrm{Vol}(X)ABT_0 = -2\,\mathrm{Vol}(X)i\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{ds}{C(s)}AB\left[V(\phi) - V_A\right]. \tag{3.85}$$

Based on the foregoing results, we observe that for this metric, both Hamiltonian factorizations lead to the same expression for the transition amplitudes, with the exception of the exponents appearing in the tension term in (3.85) as compared to (3.72). Thus, for the first quantum correction we have the term

$$\begin{aligned}\nabla^2\mathcal{V} = G^{MN}\frac{\partial^2 f}{\partial\Phi^M\partial\Phi^N} &= 2G^{AB}\frac{\partial^2 f}{\partial A\partial B} + G^{\phi\phi}\frac{\partial^2 f}{\partial\phi^2} \\ &= \left(-2V + V^{(2)}\right).\end{aligned} \tag{3.86}$$

Substituting these results into the general expression given by (2.33), we obtain the first quantum correction:

$$\Gamma_1 = \frac{\mathrm{Vol}(X)}{2}\left(\frac{V_B^{(2)}}{V_B} - \frac{V_A^{(2)}}{V_A}\right)\ln(A)\Big|_{A_0}^{\bar{A}+\delta A} - \mathrm{Vol}^2(X)\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{ds}{C^2(s)}\left(\tilde{V} - \tilde{V}_A\right), \tag{3.87}$$

where we have defined the terms $\tilde{V} = 2V - V^{(2)}$ and $\tilde{V}_A = \tilde{V}(V(\phi = \phi_A))$. Proceeding to the second quantum correction, the evaluation yields

$$\begin{aligned}\Gamma_2 = &\frac{i\hbar\,\mathrm{Vol}(X)}{2^{7/2}}\left(W_B - W_A\right)\left(\frac{1}{A^2}\right)\Big|_{A_0}^{\bar{A}-\delta A} \\ &+ \frac{i\hbar\,\mathrm{Vol}^3(X)}{2}\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{ds}{C^3(s)}\left(\frac{1}{AB}\right)(\bar{V} - \bar{V}_A) \\ &+ \frac{i\hbar\,\mathrm{Vol}^5(X)}{2}\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{ds}{C^5(s)}\left(\frac{1}{AB}\right)\left(\bar{\bar{V}} - \bar{\bar{V}}_A\right),\end{aligned} \tag{3.88}$$

where the auxiliary functions are defined as follows

$$W = \frac{-\left(V^{(4)} - 2V^{(2)}\right)}{V^{1/2}\left(2V^2 - V^{(1)2}\right)^{1/2}} - \frac{V^{1/2}\left(V^{(3)} - 2V^{(1)}\right)^2}{2\left(2V^2 - V^{(1)2}\right)^{3/2}}, \tag{3.89}$$

$$\bar{V} = V^{(4)} - 2V^{(2)}, \tag{3.90}$$

and

$$\bar{\bar{V}} = \left(V^{(3)} - 2V^{(1)}\right)^2. \tag{3.91}$$

Consequently, based on the derived expressions, it is evident that the results corresponding to the flat case are recovered identically, given the relationship $A = b_0B$. This finding demonstrates that within the anisotropic Bianchi Type I scenario, access to the initial singularity is preserved only when the Hamiltonian constraint is treated without any additional factorization.

3.4 Transitions for a Bianchi Type III Metric

In this section, we extend the analysis of anisotropic cosmologies by following an analogous procedure for the Bianchi Type III metric. This metric allows us to explore the effects of spatial anisotropy on the vacuum transition probability. The line element is defined as

$$ds^2 = -N(t)dt^2 + A(t)^2dx^2 + B(t)^2e^{-2\alpha x}dy^2, \tag{3.92}$$

where α is a constant parameterizing the anisotropy. Consequently, the square root of the metric determinant is given by $\sqrt{-g} = NABe^{-\alpha x}$. The corresponding Ricci scalar is calculated as

$$R = \frac{-2}{A^2BN^3}\left\{B\left(\alpha^2N^3 + A\dot{A}\dot{N} - AN\ddot{A}\right) + A[A\dot{B} - N(\dot{A}\dot{B} + A\ddot{B})]\right\}. \tag{3.93}$$

Substituting these geometric quantities into the general action given in (3.1), and integrating over the spatial coordinates, the action can be rewritten in the minisuperspace form

$$S = \mathrm{Vol}(X)\int dt\left(-\frac{\dot{A}\dot{B}}{N} - \frac{\alpha^2BN}{A} + \frac{AB\dot{\phi}^2}{2N} - NABV\right). \tag{3.94}$$

In this context, the spatial volume factor $\mathrm{Vol}(X)$ incorporates the exponential dependence on the coordinate x, defined as

$$\mathrm{Vol}(X) = \iint e^{-\alpha x}dxdy. \tag{3.95}$$

From the action, we identify the Lagrangian of the system as

$$\mathcal{L} = -\frac{\dot{A}\dot{B}}{N} - \frac{\alpha^2BN}{A} + \frac{AB\dot{\phi}^2}{2N} - NABV. \tag{3.96}$$

The corresponding canonical momenta are derived via standard definition

$$\begin{cases} \pi_N = 0, \\ \pi_A = -\frac{\dot{B}}{N}, \\ \pi_B = -\frac{\dot{A}}{N}, \\ \pi_\phi = \frac{AB\dot{\phi}}{N}. \end{cases} \tag{3.97}$$

Using these momenta, the Hamiltonian is constructed as

$$\mathcal{H} = \frac{N}{AB}\left(-\pi_A\pi_BAB + \frac{\pi_\phi^2}{2} + A^2B^2V + \alpha^2B^2\right). \tag{3.98}$$

We observe that this Hamiltonian coincides with the general quadratic form. Now, we identify the non-zero components of the minisuperspace metric as

$$G^{MN} = \begin{pmatrix} 0 & -AB & 0 \\ -AB & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{3.99}$$

While the metric structure remains identical to the Bianchi Type I case, the function $\mathcal{V}$ is modified by the anisotropy parameter α, taking the form

$$\mathcal{V} = A^2B^2V + \alpha^2B^2 = B^2\left(A^2V + \alpha^2\right). \tag{3.100}$$

Consequently, the semiclassical transition probability Γ_0 is expressed as

$$\begin{aligned}\pm\Gamma_0 = \frac{-2\,\mathrm{Vol}(X)i}{\hbar}\Bigg\{&\int_0^{\bar{s}-\delta s}\frac{ds}{C(s)}B^2\left(A^2V_B+\alpha^2\right)\\&-\int_0^{\bar{s}-\delta s}\frac{ds}{C(s)}B^2\left(A^2V_A+\alpha^2\right)+\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{ds}{C(s)}B^2A^2\left[V(\phi)-V_A\right]\Bigg\}.\end{aligned}\tag{3.101}$$

To evaluate the first two integrals, we utilize the equation $C^2(s) = 16\,\mathrm{Vol}^2(X)A^2B^2V$ and the derived equations that relate the scale factors and the parameter s as

$$\begin{cases}\frac{dA}{ds} = \frac{\left(A^2V+\alpha^2\right)}{4\,\mathrm{Vol}(X)AV},\\ \frac{dB}{ds} = \frac{B}{4\,\mathrm{Vol}(X)}.\end{cases}\tag{3.102}$$

Solving this system yields a specific relationship between the scale factors A and B

$$B = b_0\sqrt{A^2+\frac{\alpha^2}{V}},\tag{3.103}$$

where b_0 is an integration constant. This relationship allows us to transform the integration variable from the parameter s to the scale factor A. The integral in the region of constant field becomes

$$\begin{aligned}\int\mathcal{V}\frac{ds}{C(s)} &\Rightarrow \int\sqrt{V}\sqrt{A^2+\frac{\alpha^2}{V}}dA\\&= \frac{AV\sqrt{A^2+\frac{\alpha^2}{V}}+\alpha^2\ln\left(\sqrt{A^2+\frac{\alpha^2}{V}}+A\right)}{2\sqrt{V}}.\end{aligned}\tag{3.104}$$

Substituting this result back into the expression for Γ_0, we obtain

$$\begin{aligned}\pm\Gamma_0 = \frac{-2\,\mathrm{Vol}(X)i}{\hbar}&\Bigg\{\pm\left(\frac{b_{0B}}{2\sqrt{V_B}}\right)\left[AV_B\sqrt{A^2+\frac{\alpha^2}{V_B}}+\alpha^2\ln\left(\sqrt{A^2+\frac{\alpha^2}{V_B}}+A\right)\right]\Bigg|_{A_0}^{\bar{A}-\delta A}\\&\mp\left(\frac{b_{0A}}{2\sqrt{V_A}}\right)\left[AV_A\sqrt{A^2+\frac{\alpha^2}{V_A}}+\alpha^2\ln\left(\sqrt{A^2+\frac{\alpha^2}{V_A}}+A\right)\right]\Bigg|_{A_0}^{\bar{A}-\delta A}\Bigg\}\\&+\frac{\mathrm{Vol}(X)A^2B^2T_0}{\hbar},\end{aligned}\tag{3.105}$$

where the tension term T_0 is defined by the integral over the wall width

$$\mathrm{Vol}(X)A^2B^2T_0 = -2\,\mathrm{Vol}(X)i\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{ds}{C(s)}A^2B^2\left[V(\phi)-V_J\right].\tag{3.106}$$

Now, it is possible to consider the condition $A_0 = 0$ such that the semiclassical contribution to the probability takes the form

$$
\begin{aligned}
\pm\Gamma_0 = -\frac{2\,\mathrm{Vol}(X)i}{\hbar}\Bigg\{ &\pm\left(\frac{b_{0B}}{2\sqrt{V_B}}\right)\left[\bar{A}V_B\sqrt{\bar{A}^2+\frac{\alpha^2}{V_B}}+\alpha^2\ln\left(\sqrt{\bar{A}^2+\frac{\alpha^2}{V_B}}+\bar{A}\right)\right] \\
&-\left(\frac{b_{0A}}{2\sqrt{V_A}}\right)\left[\bar{A}V_A\sqrt{\bar{A}^2+\frac{\alpha^2}{V_A}}+\alpha^2\ln\left(\sqrt{\bar{A}^2+\frac{\alpha^2}{V_A}}+\bar{A}\right)\right] \\
&\pm\frac{\alpha^2}{4}\left[\left(\frac{b_{0A}}{\sqrt{V_A}}\right)\ln\left(\frac{\alpha^2}{V_A}\right)-\left(\frac{b_{0B}}{\sqrt{V_B}}\right)\ln\left(\frac{\alpha^2}{V_B}\right)\right]\Bigg\} \\
&+\frac{\mathrm{Vol}(X)A^2B^2T_0}{\hbar}.
\end{aligned}
\tag{3.107}
$$

To visualize the consequences of anisotropy in $(2+1)$ dimensions, we analyze the transition probability $P(A \to B) = \exp[-2\,\mathrm{Re}(\Gamma)]$ derived from (3.107). We vary the parameter α, which measures the degree of anisotropy. By selecting the negative sign for the sum of contributions, we ensure a well-behaved probability. Figure 3.1 illustrates the transition probability as a function of the

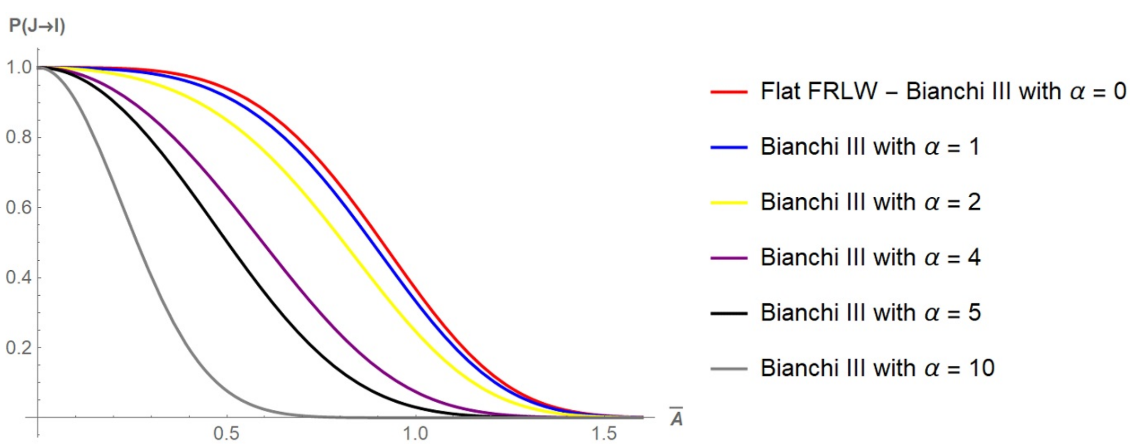

Figure 3.1: Transition probability in units such that $\frac{2\,\mathrm{Vol}(X)}{\hbar} = 1$, with $V_A = 100$, $V_B = 10$ and $T_0 = 1$ for the Bianchi Type III metric. The curves correspond to different values of the anisotropy parameter α. $\alpha = 0$ (Red line), $\alpha = 1$ (Blue line), $\alpha = 2$ (Yellow line), $\alpha = 4$ (Purple line), $\alpha = 5$ (Black line), $\alpha = 10$ (Gray line).

scale factor $\bar{A}$, while Figure 3.2 displays the probability as a function of the tension T_0. It is worth noting that in the limit $\alpha \to 0$, imposed alongside the condition $A = B$, the results corresponding to the flat FLRW metric are recovered.

We want to emphasize that this behavior is analogous to that obtained in [51] for the $(3+1)$ dimensional case. Finally, we address the case of negative potentials. To maintain real-valued solutions for the geometry, it is necessary to invert the relationship between A and B in (3.103).

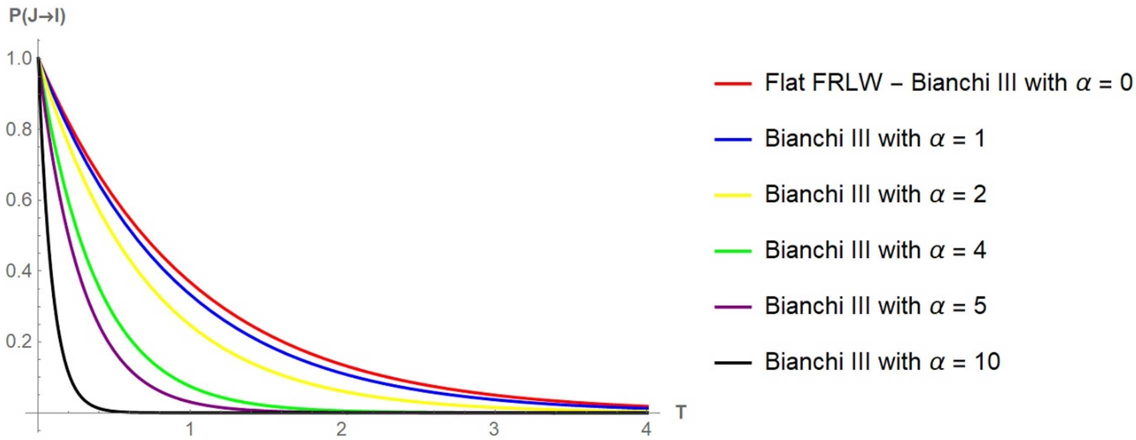

Figure 3.2: Transition probability in units such that $\frac{2\,\mathrm{Vol}(X)}{\hbar} = 1$, with $V_A = 100$, $V_B = 10$ and $\bar{A} = 1$ for the Bianchi Type III metric.$\alpha = 0$ (Red line), $\alpha = 1$ (Blue line), $\alpha = 2$ (Yellow line), $\alpha = 4$ (Purple line), $\alpha = 5$ (Black line), $\alpha = 10$ (Gray line).

This inversion leads to the following expression for the probability

$$\begin{aligned}
\pm\Gamma_0 = &-\frac{2\,\mathrm{Vol}(X)i}{\hbar}\left\{\pm\left(\frac{b_{0A}}{2\sqrt{V_A}}\right)\left[\bar{B}V_A\sqrt{\bar{B}^2-\frac{\alpha^2}{V_A}}+\alpha^2\ln\left(\sqrt{\bar{B}^2-\frac{\alpha^2}{V_A}}+\bar{B}\right)\right]\right.\\
&\mp\left(\frac{b_{0B}}{2\sqrt{V_B}}\right)\left[\bar{B}V_B\sqrt{\bar{B}^2-\frac{\alpha^2}{V_B}}+\alpha^2\ln\left(\sqrt{\bar{B}^2-\frac{\alpha^2}{V_B}}+\bar{B}\right)\right]\\
&\left.\pm\frac{\alpha^2}{4}\left[\left(\frac{b_{0A}}{\sqrt{V_A}}\right)\ln\left(\frac{\alpha^2}{V_A}\right)-\left(\frac{b_{0B}}{\sqrt{V_B}}\right)\ln\left(\frac{\alpha^2}{V_B}\right)\right]\right\}\\
&+\frac{\mathrm{Vol}(X)(\bar{B}^2-\frac{\alpha^2}{V_B})B^2T_0}{\hbar}.
\end{aligned} \tag{3.108}$$

Plotting this probability as a function of $\bar{B}$ yields the behavior shown in Figure 3.3. Thus, for the determination of the first quantum correction, we first identify the relevant term

$$\begin{aligned}
\nabla^2\mathcal{V} = G^{MN}\frac{\partial^2\mathcal{V}}{\partial\Phi^M\partial\Phi^N} &= 2G^{AB}\frac{\partial^2\mathcal{V}}{\partial A\partial B}+G^{\phi\phi}\frac{\partial^2\mathcal{V}}{\partial\phi^2}\\
&=\left(-8A^2B^2V+A^2B^2V^{(2)}\right).
\end{aligned} \tag{3.109}$$

Substituting this result into the general expression given by (2.33) and performing the necessary integrations, we obtain the explicit form for Γ_1. It is noteworthy that the logarithmic arguments in the regions of constant field now explicitly depend on the anisotropy parameter α, reflecting the specific geometry of the Bianchi Type III metric

$$\begin{aligned}
\Gamma_1 = &\frac{\mathrm{Vol}(X)}{8}\left[\left(8-\frac{V_A^{(2)}}{V_A}\right)\ln\left(\alpha^2+\bar{A}^2V_A\right)-\left(8-\frac{V_B^{(2)}}{V_B}\right)\ln\left(\alpha^2+\bar{A}^2V_B\right)\right]\\
&-\frac{\ln(\alpha^2)\,\mathrm{Vol}(X)}{8}\left(\frac{V_B^{(2)}}{V_B}-\frac{V_A^{(2)}}{V_A}\right)\\
&-\mathrm{Vol}^2(X)\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{ds}{C^2(s)}A^2B^2\left(\tilde{V}-\tilde{V}_A\right),
\end{aligned} \tag{3.110}$$

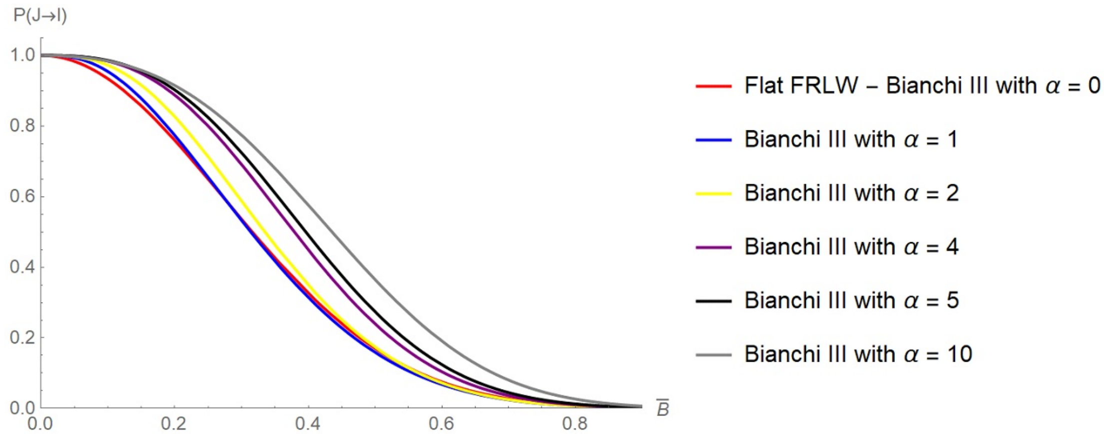

Figure 3.3: Transition probability in units such that $\frac{2\,\mathrm{Vol}(X)}{\hbar} = 1$, with $V_A = -10$, $V_B = -100$ and $T_0 = 1$ for the Bianchi Type III metric with negative potentials.$\alpha = 0$ (Red line), $\alpha = 1$ (Blue line), $\alpha = 2$ (Yellow line), $\alpha = 4$ (Purple line), $\alpha = 5$ (Black line), $\alpha = 10$ (Gray line)

where we have defined the term $\tilde{V} = 8V - V^{(2)}$. It is observed that, in contrast to the semiclassical contribution, the limit $\alpha \to 0$ fails to recover the results obtained for the flat case. Thus showing that with the inclusion of quantum corrections there may not be equivalence. Proceeding to the second quantum correction, we evaluate the higher order terms in the semiclassical expansion. This results in Γ_2, which includes contributions that are inversely proportional to α^2, and two different functional forms in the region of the wall, such that

$$\begin{aligned}\Gamma_2 =& \frac{i\hbar\,\mathrm{Vol}(X)}{32}\left[\frac{\bar{A}}{\left(\bar{A}^2 V_B + \alpha^2\right)^{1/2}\alpha^2} W_B - \frac{\bar{A}}{\left(\bar{A}^2 V_A + \alpha^2\right)^{\frac{1}{2}}\alpha^2} W_A\right] \\ &+ \frac{i\hbar\,\mathrm{Vol}^3(X)}{2}\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{ds}{C^3(s)} A^2 B^2 \left(\bar{V} - \bar{V}_A\right) \\ &+ \frac{i\hbar\,\mathrm{Vol}^5(X)}{2}\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{ds}{C^5(s)} A^4 B^4 \left(\bar{\bar{V}} - \bar{\bar{V}}_A\right),\end{aligned} \tag{3.111}$$

where the auxiliary functions $W_{A,B}$, $\bar{V}$, and $\bar{\bar{V}}$, which encapsulate the contributions from higher-order derivatives of the potential, are defined as follows

$$W_{A,B} = 64V_{A,B} - 16V_{A,B}^{(2)} + V_{A,B}^{(4)} - \frac{1}{16}\left(-512V_{A,B}^2 + 128V_{A,B}V_{A,B}^{(2)} - 8V_{A,B}^{(2)2} + V_{A,B}^{(3)2}\right), \tag{3.112}$$

$$\bar{V} = 64V - 16V^{(2)} + V^{(4)}, \tag{3.113}$$

and

$$\bar{\bar{V}} = -512V^2 + 64V^{(1)2} + 128VV^{(2)} - 8V^{(2)2} - 16V^{(1)}V^{(3)} + V^{(3)2}. \tag{3.114}$$

Here, we observe once again that, enven if the amplitudes are well behaved, the recovery of the flat case from the Bianchi Type III metric is not possible once quantum corrections are taken into consideration. We also see that this factorization does not prevent the initial singularity, since $\lim_{\bar{a}\to 0} P(A \to B) = 1$.

Based on the calculations presented in this chapter, several key conclusions can be drawn. The specific factorization scheme adopted for the Hamiltonian constraint plays a pivotal role in determining the final impact of the quantum corrections. While this influence may be negligible in the calculation of the semiclassical contribution, it becomes significant when quantum corrections are taken into account. It is noteworthy that, in general, when no additional factorization is applied, the effect of the corrections is substantial: the first correction preserves the qualitative behavior but reduces the maximum probability from unity to a lower value, whereas the second correction suppresses the probability to zero at the origin. Consequently, the most probable initial size of the nucleated universe corresponds to a finite value, thereby effectively avoiding the initial singularity. Building upon this methodological exercise within the framework of $(2+1)$ dimensional gravity, we may now proceed to investigate the physically realistic $(3+1)$ dimensional case, incorporating these considerations.

Chapter 4

Transition probabilities in $3+1$ dimensions

In this chapter, we present a comprehensive study of vacuum transition probabilities, explicitly incorporating quantum corrections. Building upon the results obtained in the $(2+1)$ dimensional framework, we extend the analysis to the physically relevant case of $(3+1)$ dimensions. For the isotropic scenario, we employ the FLRW metric with positive and zero spatial curvature. Conversely, for the anisotropic case, we analyze the Bianchi III and Kantowski–Sachs metrics. Interpreting the results the results as distribution probabilities of creating universes with a given size via vacuum decay, we demonstrate that the general behavior, specifically, the consideration of corrections up to the second order, leads to the avoidance of the initial singularity. This outcome aligns with expectations derived from the analysis in lower dimension. However, we demonstrate that this resolution of the singularity is strictly achievable only within the isotropic regime. Furthermore, the specific influence of anisotropy on the transition probabilities is rigorously examined.

4.1 Transitions for a closed FLRW metric

We begin with the FLRW closed metric that describes a closed homogeneous isotropic universe with positive spatial curvature. The FLRW metric with positive curvature in $3+1$ dimensions is written as

$$ds^2 = -N^2(t)dt^2 + a^2(t)\left(dr^2 + \sin^2 r d\Omega_2^2\right), \tag{4.1}$$

where $r \in [0, \pi]$, $d\Omega_2^2$ the metric of the sphere, $a(t)$ is the scale factor and $N(t)$ is the lapse function. Considering that the scalar field coupled in (2.36) depends only on the time variable, i.e., $\phi = \phi(t)$, we obtain the Lagrangian for this system as

$$\mathcal{L} = 3N(t)a(t) - \frac{3a(t)\dot{a}(t)^2}{N(t)} + \frac{a^3(t)\dot{\phi}^2}{2N(t)} - N(t)a^3(t)V(\phi) \tag{4.2}$$

where $\dot{a}(t)$ stands for the derivative with respect to the time variable t and $V(\phi)$ is the scalar field potential. In a standard way, we obtain the conjugate canonical momenta as

$$\pi_N = 0, \quad \pi_a = -\frac{6a\dot{a}}{N}, \quad \pi_\phi = \frac{a^3\dot{\phi}}{N} \tag{4.3}$$

leading us to the Hamiltonian constraint

$$\mathcal{H} = N\left[\frac{\pi_\phi^2}{2a^3} - \frac{\pi_a^2}{12a} - 3a + a^3V\right] \simeq 0. \tag{4.4}$$

As always, since the canonical momentum with respect to N vanishes, we can ignore the prefactor and focus only on the term inside brackets in the last expression, then by comparing it with the general form (1.38), we see that for this metric the set of variables is $\left\{\Phi^M\right\} = \{a, \phi\}$, while the metric in minisuperspace results in

$$(G^{MN}) = \left(\begin{array}{cc} -1/6a & 0 \\ 0 & 1/a^3 \end{array} \right) \tag{4.5}$$

and we identify the remaining terms as

$$\mathcal{V}(a, \phi) = -3a + a^3 V(\phi). \tag{4.6}$$

We also note that for this metric the volume of the spatial slice is given by

$$\mathrm{Vol}(X) = \int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi} \int_{r=0}^{\pi} \sin^2 r \sin\theta dr d\theta d\phi = 2\pi^2 \tag{4.7}$$

which is finite. In this case following the general method we can only choose $\Phi^i = a$ since there is only one degree of freedom coming from the metric, furthermore we can choose $a_0 = a(s=0) = 0$ since the expressions are well behaved for this value. Thus in this case the semiclassical contribution to the transition probability (2.39) takes the form

$$\begin{aligned} \Gamma_0 = \pm \frac{12\pi^2}{\hbar} &\left\{ \frac{1}{V_B} \left[\left(1 - \frac{V_B}{3} \bar{a}^2 \right)^{3/2} - 1 \right] - \frac{1}{V_A} \left[\left(1 - \frac{V_A}{3} \bar{a}^2 \right)^{3/2} - 1 \right] \right\} \\ &+ \frac{2\pi^2}{\hbar} \bar{a}^3 T_0. \end{aligned} \tag{4.8}$$

This result was derived in [50,51] and coincides with the one obtained with the Euclidean approach. We note from this resut that $\lim_{\bar{a}\to 0} \Gamma_0 = 0$, then taking only this semiclassical contribution we will obtain that the transition probability fulfills $\lim_{\bar{a}\to 0} P(A \to B) = 1$. Therefore, interpreting the transition probabilities as probability distributions of creating universes with a given size $\bar{a}$ as it has been previously done in [50–53], we note that the semiclassical contribution implies that the most possible scenario is that the universe is created at the spatial singularity.

Let us continue with the first quantum correction, that is the term of order $\mathcal{O}(\hbar)$ in the WKB expansion. The general expression for this term is written in (2.41). For this metric we find that

$$\nabla^2 \mathcal{V} = V^{(2)} - V. \tag{4.9}$$

Theferore, substituting in (2.41) we obtain

$$\Gamma_1 = \pi^2 \left[\left(\frac{V_B^{(2)}}{V_B} - 1 \right) \ln\left(1 - \bar{a}^2 V_B\right) - \left(\frac{V_A^{(2)}}{V_A} - 1 \right) \ln\left(1 - \bar{a}^2 V_A\right) \right] + 2\pi^2 T_1. \tag{4.10}$$

We note that in this case there only appears one tension term, since both expressions for the tension terms in the general form are equivalent, thus the first quantum correction only adds one independent parameter to the transition probability. Moreover we note that $\lim_{\bar{a}\to 0} \Gamma_1 = 2\pi^2 T_1$ wich is a constant. Therefore, the inlcusion of the first quantum correction will not alter the fact that the point with the biggest probability is the spatial singularity ($\bar{a} = 0$) but it reduces the probability in that point.

Let us now move on to the second quantum correction. In this case we obtain

$$\begin{aligned} \nabla^2 \left(\nabla^2 \mathcal{V}\right) &= \frac{1}{a^3} \left(V^{(4)} - V^{(2)} \right), \\ \left(\nabla \left(\nabla^2 \mathcal{V}\right)\right)^2 &= \frac{1}{a^3} \left(V^{(3)} - V^{(1)} \right)^2. \end{aligned} \tag{4.11}$$

then, for this metric we have

$$\frac{\mathrm{Vol}(X)\hbar}{4\sqrt{2}}\int_{\Phi_0^i}^{\bar{\Phi}^i}\frac{\nabla^2\left(\nabla^2\mathcal{V}\right)}{\nabla^i\mathcal{V}}\sqrt{\frac{\mathcal{V}}{(\nabla\mathcal{V})^2}}\Bigg|_{\phi=\phi_B}d\Phi^i=\pi^2\hbar\left(V^{(4)}-V^{(2)}\right)F(V_B,a)\Bigg|_{a_0}^{\bar{a}}, \tag{4.12}$$

$$\frac{\mathrm{Vol}(X)\hbar}{8\sqrt{2}}\int_{\Phi_0^i}^{\bar{\Phi}^i}\frac{\left(\nabla\left(\nabla^2\mathcal{V}\right)\right)^2}{\nabla^i\mathcal{V}}\sqrt{\left(\frac{\mathcal{V}}{(\nabla\mathcal{V})^2}\right)^3}\Bigg|_{\phi=\phi_B}=\pi^2\hbar(V^{(3)})^2G(V_B,a)\Bigg|_{a_0}^{\bar{a}}, \tag{4.13}$$

where we have defined the functions

$$\begin{aligned}F(V,a)=\int\frac{\left(1-\frac{V}{3}\bar{a}^2\right)^{1/2}}{a\left(1-V\bar{a}^2\right)^2}da=-\frac{\sqrt{1-\frac{V}{3}a^2}}{2\left(-1+Va^2\right)}+\frac{5}{2\sqrt{6}}\operatorname{arctanh}\left(\frac{\sqrt{3-Va^2}}{\sqrt{2}}\right)\\-\operatorname{arctanh}\left[\sqrt{1-\frac{V}{3}a^2}\right],\end{aligned} \tag{4.14}$$

$$\begin{aligned}G(V,a)=\int\frac{a\left(1-\frac{V}{3}\bar{a}^2\right)^{3/2}}{(1-V\bar{a}^2)^4}da=\frac{1}{576\sqrt{3V}}\Bigg[-\frac{2\sqrt{3-Va^2}\left(63-34Va^2+3V^2a^4\right)}{(-1+Va^2)^3}\\-3\sqrt{2}\operatorname{arctanh}\left(\frac{\sqrt{3-Va^2}}{\sqrt{2}}\right)\Bigg].\end{aligned} \tag{4.15}$$

We note that the $G(V,a)$ function is well behaved if we take the limit $a\to 0$. On the other hand the third term of the $F(V,a)$ function diverges in this limit. However, we note that this limit is independent of V, therefore we can eliminate this divergence in the transition probability by imposing the condition

$$V_B^{(4)}-V_B^{(2)}=V_A^{(4)}-V_A^{(2)}, \tag{4.16}$$

in this way we can still choose $a_0=0$ in order to have access to the initial spatial singularity. Furthermore for this metric from the eleven possible tension terms only one remains since all the nonzero terms have the same dependence on $\bar{a}$, thus we finally obtain that the second quantum correction is written as

$$\begin{aligned}\Gamma_2=\pm\,\pi^2\hbar\Big\{\left(V_B^{(4)}-V_B^{(2)}\right)\left[F\left(V_B,\bar{a}\right)-F\left(V_A,\bar{a}\right)\right]-\left(V_B^{(3)}\right)^2\left[G\left(V_B,\bar{a}\right)-G\left(V_B,0\right)\right]\\+\left(V_A^{(3)}\right)^2\left[G\left(V_A,\bar{a}\right)-G\left(V_A,0\right)\right]\Big\}+\frac{2\pi^2\hbar}{\bar{a}^3}T_2.\end{aligned} \tag{4.17}$$

We note that once again, the second quantum correction only adds one more independent parameter tension term. From this result we also note that the limit $\lim_{\bar{a}\to 0}\Gamma_2$ will diverge because of the tension term. Thus, choosing appropriately the sign of (2.39) we will obtain that taking into account up to second order in the quantum corrections the transition probability fulfills $\lim_{\bar{a}\to 0}P(A\to B)=0$. Therefore, the second order quantum correction implies that the most probable size of the universe to be created is a finite non zero value of the scale factor. In this way, the quantum correction terms leads to a result that avoids the spatial singularity.

Let us remark from (4.8) that the semiclassical contribution Γ_0 is well behaved for all values of the potentials, it can be complex for positive values of the potential minima but this not a problem since we take only the real part always. Nevertheless we see from (4.10) that Γ_1 have a divergence in $\bar{a}^2=V_{A,B}^{-1}$ which can occur for positive values of the potential minima. Furthermore from (4.17) we note that Γ_2 will also have a divergence appearing in $\bar{a}^2=\frac{5}{V_{A,B}}$, which can also appear for positive values of the potential minima. In this cases, the transition probability will only be well defined up to an upper limit. On the other hand, we note that for negative potential minima everything is well defined without any issue. Therefore positive values of the potential minima will imply some additional restrictions for the validity of the transition probabilities. Moreover, in order to have a well defined second quantum correction term we need to impose additional restrictions on the higher derivatives of the potential.

In order to explicitly visualize the effect of the first and second order quantum corrections for all values of the scale factor, we plot in Figure 4.1 the transition probability (2.28) using the results for this metric, that is using eq. (4.8) for the semiclassical contribution, eq. (4.10) for the first quantum correction and eq. (4.17) for the second order quantum correction. We choose units in which $\hbar = 1$, we also choose $V_B = -1.5$, $V_A = -1$, $\frac{V_B^{(2)}}{V_B} - 1 = \frac{V_A^{(2)}}{V_A} - 1 = 0.05$, $V_B^{(4)} - V_B^{(2)} = -0.005$, $V_B^{(3)} = V_A^{(3)} = 0.1$, $T_0 = 0.005$, $T_1 = 5 \times 10^{-4}$ and $T_2 = 10^{-6}$. In order to have a well defined transition probability we choose the plus sing in the left hand side of (2.39) and the minus sign in the right of (4.8) which corresponds to the minus sign in (4.17) as well. We note that the result with the semiclassical contribution only has a maximum value on the spatial singularity and as $\bar{a}$ increases, the probability decreaeses. The result including the first quantum correction does not change the overall shape of the curve, it only reduces the overall probability and it make it fall faster. However, as we have previously seen, when the second quantum correction is taken into account as well, the shape of the curve is changed in the ultraviolet (small values of the scale factor), in such a way that the maximum value of the transition probability is no longer in the spatial singularity, it is instead located at a small nonzero value of the scale factor. From this point, the same behaviour is encountered as in the other two results in the infrared, that is as the scale factor increases, the probability decreases. Thus, the quantum corrections are only relevant on the ultraviolet as expected.

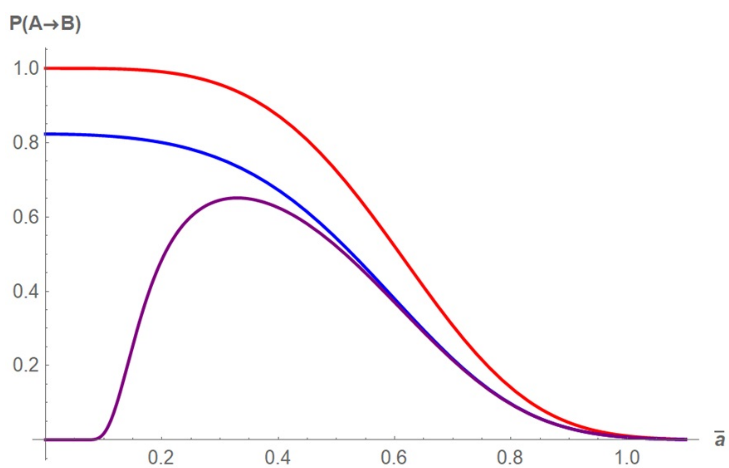

Figure 4.1: Transition probability for the positive FLRW metric in units such that $\hbar = 0.1$, choosing $V_B = -2$, $V_A = -1$, $\frac{V_B^{(2)}}{V_B} - 1 = \frac{V_A^{(2)}}{V_A} - 1 = 0.5$, $V_B^{(4)} - V_B^{(2)} = -0.05$, $V_B^{(3)} = V_A^{(3)} = 0.1$, $T_0 = 1$, $T_1 = 5 \times 10^{-4}$, $T_2 = 10^{-6}$. We plot the results with the semiclasical contribution Γ_0 (red line), including the first quantum correction $\Gamma_0 + \Gamma_1$ (blue line) and including the second quantum correction $\Gamma_0 + \Gamma_1 + \Gamma_2$ (purple line).

4.2 Transitions for a flat FLRW metric

Let us consider now the FLRW metric with zero spatial curvature. This metric will be important in the following since it represents the isotropic limit of the Bianchi III metric. We can write this metric in cartesian coordinates as follows

$$ds^2 = -N(t)dt^2 + a^2(t)\left[dx^2 + dy^2 + dz^2\right]. \tag{4.18}$$

As stated above, the gravitational and scalar fields depend only on the time variable t. Thus the corresponding Lagrangian is given by

$$\mathcal{L} = -\frac{3a(t)\dot{a}(t)^2}{N(t)} + \frac{a^3(t)\dot{\phi}^2}{2N(t)} - N(t)a^3(t)V(\phi) \tag{4.19}$$

and the Hamiltonian constraint is

$$\mathcal{H} = N\left[\frac{\pi_\phi^2}{2a^3} - \frac{\pi_a^2}{12a} + a^3 V\right] \simeq 0. \tag{4.20}$$

As always the N function is not dynamical, so we can focus on the terms within brackets and proceed to identify the metric in minisuperspace and the function $\mathcal{V}$. Comparing it with the general form (1.38) we see that once again the coordinates in minisuperspace are $\left\{\Phi^M\right\} = \{a, \phi\}$ with the metric

$$G^{MN} = \begin{pmatrix} -\frac{1}{6a} & 0 \\ 0 & \frac{1}{a^3} \end{pmatrix} \tag{4.21}$$

and the function $\mathcal{V}$ reads

$$\mathcal{V}(a,\phi) = a^3 V(\phi). \tag{4.22}$$

We also note that in this case the spatial volume takes the form

$$\mathrm{Vol}(X) = \iiint dxdydz. \tag{4.23}$$

In a strict sense this volume is divergent as a result of the non-compact nature of the metric. However, as we pointed out earlier we can limit the variables to a finite interval in order to obtain a finite value for this term, since it will be an overall constant we will not worry about its value and we will mantain it as an arbitrary constant that will not modify the behaviour of the transition probabilities.

Then, substituting the above identifications for this metric in eq. (2.39) we obtain

$$\Gamma_0 = \pm\frac{2i\,\mathrm{Vol}(X)}{\sqrt{3}\hbar}\left(\sqrt{V_B} - \sqrt{V_A}\right)\bar{a}^3 + \frac{\mathrm{Vol}(X)}{\hbar}\bar{a}^3 T_0. \tag{4.24}$$

We note that $\lim_{\bar{a}\to 0}\Gamma_0 = 0$, then considering only the semiclassical contribution we would obtain for the transision probability $\lim_{\alpha=0} P(A\to B) = 1$. Thus, once again, the semiclassical contribution leads to a maximum value for probability at the inital singularity.

Proceeding with the first quantum correction, we have also in this case

$$\nabla^2\mathcal{V} = V^{(2)} - V, \tag{4.25}$$

that substituting back in (2.41) we get

$$\Gamma_1 = \frac{\mathrm{Vol}(X)}{2}\left(\frac{V_B^{(2)}}{V_B} - \frac{V_A^{(2)}}{V_A}\right)\ln(a)\bigg|_{a_0}^{\bar{a}} + \frac{\mathrm{Vol}(x)}{2}T_1, \tag{4.26}$$

Therefore, as in the previous case, there only remains a single tension term, thus the first quantum correction only adds one independent constant. From this expression we also notice that the choice $a_0 = 0$ may lead to a divergence due to the logarithmic term. Therefore, in order to obtain a consistent probability we are forced to impose the condition on the second derivatives of the ptential

$$\frac{V_B^{(2)}}{V_B} = \frac{V_A^{(2)}}{V_A}, \tag{4.27}$$

therefore the first quantum correction is written finally as

$$\Gamma_1 = \frac{\mathrm{Vol}(x)}{2} T_1, \tag{4.28}$$

which is just a constant. Thus, as in the previous case the first quantum correction does not alter the overall behaviour, in particular the point with maximum probability.

Let us move on the to the computation of the second quantum correction. For this metric we also have

$$\nabla^2 \left(\nabla^2 \mathcal{V}\right) = \frac{V^{(4)} - V^{(2)}}{a^3}, \tag{4.29}$$

$$\left(\nabla \left(\nabla^2 \mathcal{V}\right)\right)^2 = \frac{\left(V^{(3)} - V^{(1)}\right)^2}{a^3}. \tag{4.30}$$

Therefore, substituing back in (2.42) and computating all the remaining terms, we obtain

$$\Gamma_2 = \pm \frac{i\hbar \,\mathrm{Vol}(X)}{2} \left[\left(W_B - W_A\right) \frac{1}{3a^3}\bigg|_{a_0}^{\bar{a}} \right] + \frac{\hbar \,\mathrm{Vol}(X)}{\bar{a}^3} T_2. \tag{4.31}$$

were we have defined

$$W = \frac{V^{(2)} - V^{(4)}}{\sqrt{3} V^{3/2}} - \frac{\left(V^{(3)}\right)^2}{3\sqrt{3} V^{5/2}}. \tag{4.32}$$

Then, for this metric we obtain once again that from the eleven possible different tension terms, only one dependence on $\bar{a}$ appears, leading to only one tension term. In this way, the second quantum correction also adds only one independent constant. Here we also note that the choice $a_0 = 0$ will lead to a divergence in the first term. However, for positive values of the potential minima we note that the first term never contributes to the transition probability after taking the real part. Therefore, for positive potentials the second quantum correction takes simply the form

$$\Gamma_2 = \frac{\mathrm{Vol}(X)\hbar}{\bar{a}^3} T_2. \tag{4.33}$$

On the other hand, for negative potential minima, this divergence can be eliminated by imposing the constraint

$$W_A = W_B. \tag{4.34}$$

Then, the negative potential minima leads to an additional constraint on the higher derivative terms of the potential, but it takes the same form as in the previous case. In any case, we note that $\lim_{\alpha=0} \Gamma_2$ will diverge. Thus by choosing the proper signs, we will obtain that $\lim_{\bar{a}\to 0} P(A \to B) = 0$ as in the previous section.

We can plot the transition probability for this metric considering the semiclassical contribution (4.24), the first quantum correction (4.28) and the second quantum correction (4.33). In this case, we obtain the same general behaviour as the one encountered for the positive FLRW metric in Figure 4.1 in the previous section. Therefore, for this metric the second quantum corrrection will also lead to an avoidance of the initial singularity.

4.3 Transitions for a Bianchi III metric

Now that we have completed the study of the FLRW metrics, let us move on to consider metrics describing homogeneous but anisotropic universes. We will begin by considering the Bianchi III metric in the present section. In a local set of coordinates we can write this metric in the following form [174–176]

$$ds^2 = -N^2(t)dt^2 + A^2(t)dx^2 + B^2(t)e^{-2\alpha x}dy^2 + C^2(t)dz^2 \tag{4.35}$$

where $\alpha \neq 0$ is a constant measuring the amount of anisotropy. We see that the isotropy limit is performed by taking $A(t) = B(t) = C(t)$ and $\alpha \to 0$ and results in the flat FLRW metric. Furthermore, if we consider different values for the scale factors $A(t)$, $B(t)$ and $C(t)$ and take $\alpha \to 0$ we will obtain the anisotropic Bianchi I metric, as explicitly show for $(2+1)$ dimensions.

Let us consider now as usual a homogeneous scalar field coupled to gravity with the metric above, the Lagrangian takes the form

$$\begin{aligned}\mathcal{L} = &-\frac{1}{N(t)}(\dot{A}(t)\dot{B}(t)C(t) + \dot{A}(t)\dot{C}(t)B(t) + \dot{B}(t)\dot{C}(t)A(t)) - \frac{\alpha^2}{A(t)}N(t)B(t)C(t)\\ &+ \frac{\dot{\phi}^2}{2N(t)}A(t)B(t)C(t) - V(\phi)N(t)A(t)B(t)C(t).\end{aligned} \tag{4.36}$$

The canonical momenta are

$$\begin{aligned}&\pi_N = 0, \quad \pi_A = -\frac{1}{N}(\dot{B}C + \dot{C}B), \quad \pi_B = -\frac{1}{N}(\dot{A}C + \dot{C}A)\\ &\pi_C = -\frac{1}{N}(\dot{A}B + \dot{B}A), \quad \pi_\phi = \frac{\dot{\phi}}{N}ABC\end{aligned} \tag{4.37}$$

then, the Hamiltonian constraint takes the form

$$\begin{aligned}\mathcal{H} = N\Bigg[&\frac{A}{4BC}\pi_A^2 + \frac{B}{4AC}\pi_B^2 + \frac{C}{4AB}\pi_C^2 - \frac{1}{2C}\pi_A\pi_B - \frac{1}{2B}\pi_A\pi_C - \frac{1}{2A}\pi_B\pi_C\\ &+\frac{\pi_\phi^2}{2ABC} + \frac{\alpha^2 BC}{A} + V(\phi)ABC\Bigg] \simeq 0.\end{aligned} \tag{4.38}$$

Comparing with the general form (1.37), we see that the coordinates on minisuperspace are $\left\{\Phi^M\right\} = \{A, B, C, \phi\}$. Moreover the metric is written as

$$\left(G^{MN}\right) = \frac{1}{2ABC}\begin{pmatrix} A^2 & -AB & -AC & 0\\ -AB & B^2 & -BC & 0\\ -AC & -BC & C^2 & 0\\ 0 & 0 & 0 & 2\end{pmatrix} \tag{4.39}$$

and the function $\mathcal{V}$ reads

$$\mathcal{V}(A, B, C, \phi) = ABC\left(V(\phi) + \frac{\alpha^2}{A^2}\right). \tag{4.40}$$

We also note that in this case the volume of X is given by

$$\mathrm{Vol}(X) = \iiint e^{-\alpha x}dxdyxdz \tag{4.41}$$

which again is finite only if we restrict to a finite interval in y and z but we will consider it as an arbitrary constant. In [51] the semiclassical contribution to the transition probability was studied for this metric. However, in that work a convenient factorization was used to obtain a result consistent in the case of a vanishing potential. In this case it will be more convenient to consider the Hamiltonian constraint without any factorization, as suggested by the results obtained for $(2+1)$ dimensions. The dependence of the results on a particular factorization for Bianchi III metric in $(3+1)$ is explored in the Appendix C.

We note that for this metric we have more than one variable on the minisuperspace in addition to the scalar field. Thus, as it was stated in the general method in Section 2 these variables will be related as a consequence of the semiclassical expansion. In particular, in the region where the scalar field is constant equation (2.11) leads to

$$\frac{dB}{dC} = \frac{B}{C}, \qquad \frac{dA}{dB} = \frac{A\left(V + \frac{3\alpha^2}{A^2}\right)}{B\left(B - \frac{\alpha^2}{A^2}\right)}, \tag{4.42}$$

which can be integrated to obtain

$$B = b_0 C = b_1 \frac{\left(A^2 + \frac{3\alpha^2}{V}\right)^{2/3}}{A^{1/3}}, \tag{4.43}$$

where b_0 and b_1 are integration constants. However, we can set these constant to 1 by rescaling the variables on the metric on a proper way for each of the solutions and demanding continuity on the wall at $\bar{B}$. Therefore we obtain for the region where the scalar field is constant

$$B = C = \frac{\left(A^2 + \frac{3\alpha^2}{V}\right)^{2/3}}{A^{1/3}}. \tag{4.44}$$

From this relation we note that the isotropy limit leads to $\lim_{\alpha\to 0} B = A$. Therefore, all the anisotropy will be measured by the contant α, Moreover as we pointed out earlier the limit $\alpha \to 0$ corresponds to the Bianchi I metric, thus from these relations we note that if we study the Bianchi I metric, we will be forced to obtain the flat FLRW metric and its corresponding result. Thus, as in $(2+1)$ dimensions, the Bianchi III metric is more suitable to study the effect of anisotropy.

Furthermore, we note that given $\alpha \neq 0$, the variable B will diverge as $A \to 0$, On the ther hand for big values of A, B increases with A. Thus, in this case the cosmological behaviour does not describe a spatial singularity at the beginning ($A = 0$). Instead we have in the early universe (understood as small values of A) a behaviour in which B and C start with big values (infinite in principle), then as A grows, they decrease until they reach a minimum value, from where they start growing. For positive potential minima this minimum value is nonzero, whereas for a negative potential minimum it is zero but always with a nonzero value of A. Thus, we have a phase of contraction on the B and C direction, until they reach a point where they start an expansion as A expands, that is, similar to a bounce scenario as the dimension described by A emerges[1]. We note that the size of the contraction phase before the bounce depends on the size of the values of $\frac{3\alpha^2}{V}$ and it dissapears in the isotropy limit. Let us remark that since we have two different degrees of freedom coming from the metric, namely A and B we can write the transition probabilities in terms of any of these two, however only A is single-valued in time, whereas the other two can have the same value twice given the bounce nature. For all these reasons we will consider only positive values of the potential minima and write the transition probabilities in terms of the A function in the following.

With the identifications made above for this metric, substituting back in (2.32) we obtain for the semiclassical contribution

$$\begin{aligned}\Gamma_0 = \pm \frac{2i\,\mathrm{Vol}(X)}{\hbar}&\left[\sqrt{V_B}F_{III}(V_B, A)\Big|_{A_0}^{\bar{A}} - \sqrt{V_A}F_{III}(V_A, A)\Big|_{A_0}^{\bar{A}}\right]\\ &+ \frac{Vol(X)}{\hbar}\bar{A}^{1/3}\left(\bar{A}^2 + \frac{3\alpha^2}{V_B}\right)^{4/3} T_0,\end{aligned} \tag{4.45}$$

where we have defined the function

$$F_{III}(V, A) = \int \frac{\left(A^2 + \frac{3\alpha^2}{V}\right)^{1/3}}{A^{5/3}} \sqrt{\left(A^2 + \frac{\alpha^2}{V}\right)\left(A^2 - \frac{\alpha^2}{V}\right)\left(3A^2 + \frac{5\alpha^2}{V}\right)} dA. \tag{4.46}$$

It can be shown that the Bianchi III results (4.45) coincides with the flat FLRW result (4.24) in the isotropy limit $\alpha \to 0$ as we expected.

[1] The relation between the coordinates can change if we consider a different factorization. This point is discussed in the appendix C.

Taking $A_0 = 0$ we note from the last expression that $\lim_{\bar{A}\to 0}\Gamma_0 = 0$. Thus we obtain once again that considering only the semiclassical contribution the probability will have its biggest value in $\bar{A} = 0$. However, let us remak that in this case this point does not represent a spatial singularity. Furthermore, varying the last expression with respect to α we obtain Figure 4.2, where in order to have a well-behaved probability we have choosen the minus sign in both sign ambiguities, additionally, we choose positive values for the potential minima, $V_B = 1$ and $V_A = 5$, and for the tension term $T_0 = 1$. We can see, as mentioned, that the case $\alpha = 0$ corresponds to the form shown above for the semiclassical contribution and that a general characteristic of anisotropy is to decrease the value of the transition probability as the value of α increases, being consistent with [51].

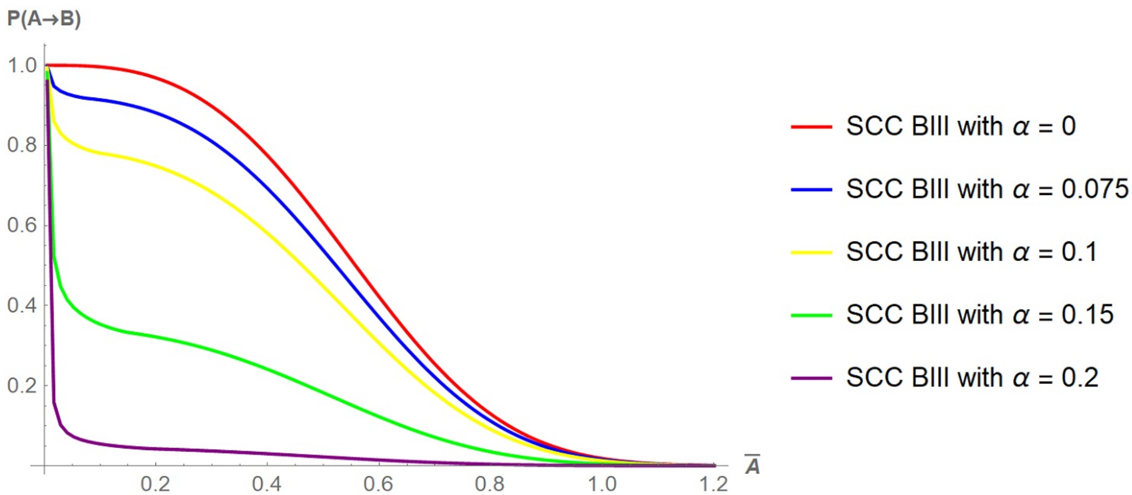

Figure 4.2: Transition probabilities for the Bianchi III metric in units such that $\hbar = 1$, choosing $V_B = 1$, $V_A = 5$, $T_0 = 1$. We plot the results of the semiclassical contribution Γ_0 for different values of α. We choose $\alpha = 0$ that corresponds to the flat FLRW case in which $\bar{A} \to \bar{a}$ (red line), $\alpha = 0.075$ (blue line), $\alpha = 0.1$ (yellow line), $\alpha = 0.15$ (green line) and $\alpha = 0.2$ (purple line).

Let us continue now with the computation of the first quantum correction, in this case we obtain

$$\nabla^2\mathcal{V} = V^{(2)} - 3V + \frac{2\alpha^2}{A^2}. \tag{4.47}$$

Then, computing the remaining terms and substituting back in eq. (2.41) we obtain for the first quantum correction

$$\begin{aligned}\Gamma_1 = \mathrm{Vol}(X)&\left[\left(\frac{V_B^{(2)}}{V_B} - \frac{11}{3}\right)\ln\sqrt{\frac{\bar{A}^2 + \frac{3\alpha^2}{V_B}}{A_0^2 + \frac{3\alpha^2}{V_B}}} - \left(\frac{V_A^{(2)}}{V_A} - \frac{11}{3}\right)\ln\sqrt{\frac{\bar{A}^2 + \frac{3\alpha^2}{V_A}}{A_0^2 + \frac{3\alpha^2}{V_A}}}\right] \\ &+ \mathrm{Vol}(X)T_1.\end{aligned} \tag{4.48}$$

We note that taking the isotropic limit $\alpha \to 0$ in the last expression we obtain the flat FLRW result of eq. (4.28). However, contrary to that case, we will not have any divergence if we take $A_0 = 0$ as long as $\alpha \neq 0$. Moreover, in order to obtain the flat FLRW result in the limit $\alpha \to 0$ we impose the same condition (4.27), thus the first quantum correction takes the form

$$\Gamma_1 = \mathrm{Vol}(X)\left\{\left(\frac{V_B^{(2)}}{V_B} - \frac{11}{3}\right)\ln\left[\sqrt{\frac{\bar{A}^2 + \frac{3\alpha^2}{V_B}}{A_0^2 + \frac{3\alpha^2}{V_B}}}\sqrt{\frac{\bar{A}^2 + \frac{3\alpha^2}{V_A}}{A_0^2 + \frac{3\alpha^2}{V_A}}}\right]\right\} + \mathrm{Vol}(X)T_1. \tag{4.49}$$

Then we now choose $A_0 = 0$, then the latter simplities to

$$\Gamma_1 = \mathrm{Vol}(X)\left(\frac{V_B^{(2)}}{V_B} - \frac{11}{3}\right)\ln\sqrt{\frac{V_B}{V_A}\left(\frac{\bar{A}^2 + \frac{3\alpha^2}{V_B}}{\bar{A}^2 + \frac{3\alpha^2}{V_A}}\right)} + \mathrm{Vol}(X)T_1. \tag{4.50}$$

However, we note that once we have chosen $A_0 = 0$ we can not longer recover the flat FLRW result (4.28) in the isotropy limit. In the isotropy limit the first quantum correction will be a constant, but the first term will contribute with a logarithmic constant term as well. Thus, the first quantum correction does not lead exactly to the flat FLRW result in the isotropy limit. Furthermore, we also note that we only obtain one tension term, thus the first quantum correction adds only one independent constant. Moreover, we note that in order to have a well defined probability we should choose only positive values of the potential minima as we have said before. Furthermore, we also note that $\lim_{\bar{A}\to 0}\Gamma_1 = \mathrm{Vol}(X)T_1$ which is a constant, thus as in the previous cases the first quantum corrrection will not alter the behaviour near the value $\bar{A} = 0$. Furthermore, again varying with respect to α, we build up Figure 4.3, where we conserved the values for the potential minima, and choose $\frac{V_B^{(2)}}{V_B} - \frac{11}{3} = -0.005$, $T_0 = 1$, $T_1 = 0.1$. It is evident that the probability changes its maximum because of the constant limit in $\bar{A} \to 0$.

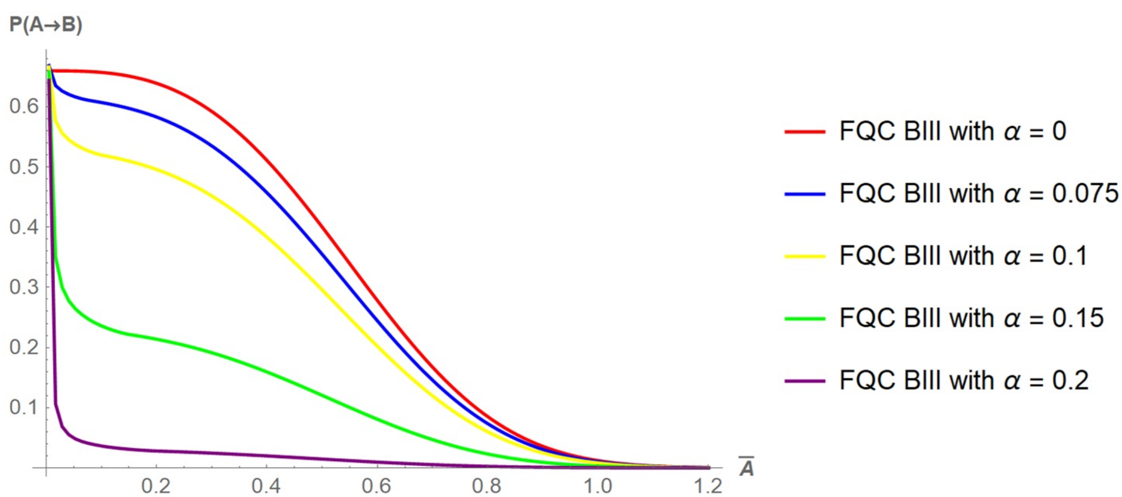

Figure 4.3: Transition probability for the Bianchi III metric in units such that $\hbar = 1$, choosing $V_B = 1$, $V_A = 5$, $\frac{V_B^{(2)}}{V_B} - \frac{11}{3} = -0.005$, $T_0 = 1$, $T_1 = 0.1$. We plot the results of the semiclassical contribution plus the first quantum correction (FQC), $\Gamma_0 + \Gamma_1$, varying the value of α; we have the cases $\alpha = 0$ (red line), $\alpha = 0.075$ (blue line), $\alpha = 0.1$ (yellow line), $\alpha = 0.15$ (green line) and $\alpha = 0.2$ (purple line).

Finally, for the second correction we obtain in this case

$$\nabla^2\left(\nabla^2\mathcal{V}\right) = \frac{V^{(4)} - 3V^{(2)} + \frac{6\alpha^2}{A^2}}{ABC}, \tag{4.51}$$

$$\left[\nabla\left(\nabla^2\mathcal{V}\right)\right]^2 = \frac{(V^{(3)} - 3V^{(1)})^2 + \frac{8\alpha^4}{A^4}}{ABC}, \tag{4.52}$$

Then, computing the remaining terms in eq. (2.42) we obtain for the second quantum correction

$$\begin{aligned}\Gamma_2 = &\pm \frac{i\hbar\,\mathrm{Vol}(X)}{2}\left[\frac{1}{V_B^{3/2}}H_{III}(V_B,A)\Big|_{A_0}^{\bar{A}} - \frac{1}{V_A^{3/2}}H_{III}(V_A,A)\Big|_{A_0}^{\bar{A}}\right]\\ &+ \frac{\mathrm{Vol}(X)\hbar}{\bar{A}^{1/3}\left(\bar{A}^2+\frac{3\alpha^2}{V_B}\right)^{4/3}}T_2.\end{aligned} \tag{4.53}$$

where the H_{III} function is defined as

$$\begin{aligned}H_{III}(V,A) = &\int \frac{dA}{A^{1/3}\left(A^2+\frac{3\alpha^2}{V}\right)^{7/3}}\sqrt{\frac{A^2+\frac{\alpha^2}{V}}{(A^2-\frac{\alpha^2}{V})(3A^2+\frac{5\alpha^2}{V})}}\\ &\times\left[6\alpha^2+\left(V^{(4)}-3V^{(2)}\right)A^4+\frac{((V^{(3)})^2A^4+8\alpha^2)\left(A^2+\frac{\alpha^2}{V}\right)}{V\left(A^2-\frac{\alpha^2}{V}\right)\left(3A^2+\frac{5\alpha^2}{V}\right)}\right].\end{aligned} \tag{4.54}$$

As in the previous case we note that the first term has an overall i, thus if the function is always real for positive potentials, this term will not contribute. Furthermore we note that once again only one tension term is added from the eleven possible because the nonzero terms have the same depende with A. However, if we take the isotropy limit for this result we obtain

$$\lim_{\alpha=0}\Gamma_2 = \pm\frac{i\hbar\,\mathrm{Vol}(X)}{2}\left[\left(\bar{W}_B-\bar{W}_A\right)\frac{1}{3A^3}\Big|_{A_0}^{\bar{A}}\right]+\frac{\hbar\,\mathrm{Vol}(X)}{\bar{A}^3}T_2. \tag{4.55}$$

were

$$\bar{W} = \frac{\left(3V^{(2)}-V^{(4)}\right)}{\sqrt{3}V^{3/2}} - \frac{\left(V^{(3)}\right)^2}{3\sqrt{3}V^{5/2}}, \tag{4.56}$$

which is very similar to the result for the FLRW metric in eq. (4.31). The only difference appears in the constant acompaning the second derivative on the W function, in this case it is a factor of 3, whereas for the flat FLRW metric it was just a factor of 1. This difference comes from the fact that although the FLRW metric follows from the isotropy limit $\alpha\to 0$, if we look for the definition of the canonical momenta on this case in (4.37), we note that the isotropy limit does not lead to the canonical momentum of the single scale factor of the FLRW metric in (4.3). The same occurs with the metric on superspace, thus the structure of the minisuperspace is not the same after taking the isotropy limit and we should not expect the same results in all scenarios. In particular we note that the Laplacian in the Bianchi III metric (4.47) does not lead to the Laplacian for the FLRW metric (4.47) in the isotropy limit. It is interesting that this discrepancy appears when we take into account the quantum corrections and it only change by constants, it does not change the general behaviour.

Now, by considering different values of α, and arduously exploring the expression (4.54), choosing $V_B=1$, $V_A=5$, $(V_{A,B}^{(3)})^2=0.1$, $V_{A,B}^{(4)}-3V_{A,B}^{(2)}>0$ it was noted that, in this setup, H_{III} takes only real values, in this way the first term in (4.53) does not contribute to the transition probability, we only have the tension term. In this manner, by choosing $V_B=1$, $V_A=5$, $\frac{V_B^{(2)}}{V_B}-\frac{11}{3}=-0.005$, $T_0=1$, $T_1=0.1$, $T_2=0.05$ we have in Figure 4.4 the transition probabilities considering up to second order quantum corrections.

Furthermore, we note that in the general case we have for this metric that $\lim_{\bar{A}\to 0}\Gamma_2$ will diverge, thus, making the probability vanish on this limit after choosing the appropriate signs. Therefore, we have obtained that the behaviour of the transition probability for the Bianchi III metric is in general the same as for the FLRW metrics, that is, the semiclassical contribution leads to a maximum value at the origin of $\bar{A}$, the first quantum correction reduces the probability

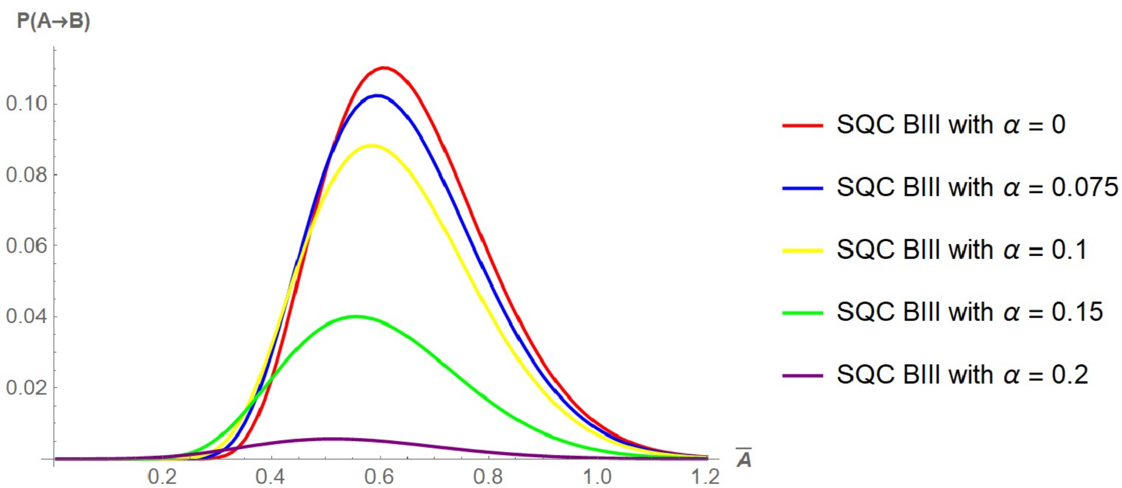

Figure 4.4: Transition probability for the Bianchi III metric in units such that $\hbar = 1$, choosing $V_B = 1$, $V_A = 5$, $\frac{V_B^{(2)}}{V_B} - \frac{11}{3} = -0.005$, $T_0 = 1$, $T_1 = 0.1$, $T_2 = 0.05$. We plot the results of the semiclassical contribution plus the first and second quantum corrections (SQC), $\Gamma_0 + \Gamma_1 + \Gamma_2$, varying the value of α; we have the cases $\alpha = 0$ (red line), $\alpha = 0.075$ (blue line), $\alpha = 0.1$ (yellow line), $\alpha = 0.15$ (green line) and $\alpha = 0.2$ (purple line).

but does not change the overall shape and the second quantum correction leads to a vanishing probability in this point. However, as we pointed out earlier for this metric this point does not represents a spatial singularity. What is being avoided in this case is the situation where one dimension is abscent an the other two are infinite in size. We could try different factorizations looking for a scenario that allows us to have access to a spatial singularity in this anisotropic metric looking for a description where the second quantum correction avoids such singularity. However, as we will show in the appendix C this scenario does not exist. Therefore, we conclude that the avoidance of the initial singularity due to quantum corrections is only possible in the isotropic case.

4.4 Transitions for a Kantowski-Sachs metric

Finally, we will consider the Kantowski-Sachs metric. This metric describes an anisotropic universe or the interior of a Schwarzschild black hole. Following the parametrization proposed by Misner [160] we can write this metric in the form

$$ds^2 = -N^2(t)dt^2 + e^{2\sqrt{3}\beta(t)}dr^2 + e^{-2\sqrt{3}(\beta(t)+\Omega(t))}\left[d\theta^2 + \sin^2(\theta)d\psi^2\right] \tag{4.57}$$

with $0 \leq \theta \leq \pi$ and $0 \leq \psi \leq 2\pi$. Let us define for simplicity the functions $\gamma(t) = e^{\sqrt{3}\beta(t)}$ and $\sigma(t) = e^{-\sqrt{3}\Omega(t)}$, then the metric is written as

$$ds^2 = -N^2(t)dt^2 + \gamma^2(t)dr^2 + \frac{\sigma^2(t)}{\gamma^2(t)}\left[d\theta^2 + \sin^2\theta d\psi^2\right] \tag{4.58}$$

Considering once again a homogeneous scalar field the Lagrangian takes the form

$$\mathcal{L} = \frac{\sigma^2(t)}{\gamma^3(t)N(t)}\dot{\gamma}^2 - \frac{\dot{\sigma}^2}{\gamma(t)N(t)} + N(t)\gamma(t) + \left[\frac{\dot{\phi}^2}{2N(t)} - N(t)V(\phi)\right]\frac{\sigma^2(t)}{\gamma(t)} \tag{4.59}$$

and the Hamiltonian constraint turns out to be

$$\mathcal{H} = N\left[\frac{\gamma^3}{4\sigma^2}\pi_\gamma^2 - \frac{\gamma}{4}\pi_\sigma^2 + \frac{\gamma}{2\sigma^2}\pi_\phi^2 + \frac{\sigma^2}{\gamma}V(\phi) - \gamma\right] \simeq 0. \tag{4.60}$$

Once more, we can focus only on the term inside brackets, and comparing it with the general form (1.37), we observe that the coordinates defining the minisuperspace are $\left\{\Phi^M\right\} = \{\gamma, \sigma, \phi\}$. Thus, the metric is

$$G^{MN} = \begin{pmatrix} \frac{\gamma^3}{2\sigma^2} & 0 & 0 \\ 0 & -\frac{\gamma}{2} & 0 \\ 0 & 0 & \frac{\gamma}{\sigma^2} \end{pmatrix} \tag{4.61}$$

and the function $\mathcal{V}$ is given by

$$\mathcal{V}(\gamma, \sigma, \phi) = \frac{\sigma^2}{\gamma} V(\phi) - \gamma. \tag{4.62}$$

We also have in this case that the volume of the saptial slice X reads

$$\mathrm{Vol}(X) = \int_r \int_{\theta=0}^{\pi} \int_{\psi=0}^{2\pi} \sin\theta dr d\theta d\psi = 4\pi \int dr, \tag{4.63}$$

which is finite only if we limit to a finite interval on r, since the spatial slice is again not compact in this scenario. Thus we will consider it as an overall arbirary contant as in the previous cases.

In order to obtain a consistent system of equations we need to consider nonzero values for the potential minima. Therefore for the region of constant scalar field, the relations (2.11) leads in this case to the differential equation

$$2\sigma V d\gamma - \gamma \left(\frac{\gamma^2}{\sigma^2} + V \right) d\sigma = 0 \tag{4.64}$$

Integration of this expression leads to the relation

$$\gamma^2 = \frac{\sigma^2 V}{1 - c\sigma} \tag{4.65}$$

where c is an integration constant. We note that by definition γ and σ are positive functions, therefore c has to fulfill the condition

$$\frac{V}{1 - c\sigma} > 0, \tag{4.66}$$

which depends on the value of V (either V_A or V_B) and the possible values that σ can have. From this expression we note that $\lim_{\sigma\to 0} \gamma = 0$ but $\lim_{\sigma\to 0} \frac{\sigma^2}{\gamma^2} = \frac{1}{V}$. Therefore, we note from the form of the metric (4.58) that the limit $\sigma \to 0$ leads to the vanishing of the radial component but not of the angular part, thus once again we will not have access to a spatial singularity.

Computing the remaining terms and substituing back in (2.39) we obtain

$$\Gamma_0 = \pm \frac{\mathrm{Vol}(X) i}{\hbar} \left[c_B F_{KS}\left[c_B, \sigma\right] \Big|_{\sigma_0}^{\bar{\sigma}} - c_A F_{KS}\left[c_A, \sigma\right] \Big|_{\sigma_0}^{\bar{\sigma}} \right] + \frac{\mathrm{Vol}(X)}{\hbar} \frac{\bar{\sigma} T}{\sqrt{V_B}} \sqrt{1 - c_B \bar{\sigma}}, \tag{4.67}$$

where we have defined the function

$$\begin{aligned} F_{KS}[c, x] &= \int \frac{\sqrt{4 - 3cx}}{1 - cx} x dx \\ &= -\frac{2}{9c^2} [\sqrt{4 - 3cx}(5 + 3cx) - 9 \operatorname{arctanh}(\sqrt{4 - 3cx})]. \end{aligned} \tag{4.68}$$

This result was first derived in [51]. We note that $\lim_{\bar{\sigma}\to 0} \Gamma_0 = 0$. Thus once again the semiclassical contribution leads to a maximum value of for the probability located at $\bar{\sigma} = 0$. Furthermore, we note that in this semiclassical contribution the tension term will be the only one that contributes after taking the real part since the integral with a constant scalar field gives always imaginary numbers.

Moving further, for the first quantum correction we obtain

$$\nabla^2 \mathcal{V} = V^{(2)} \tag{4.69}$$

Then, computing the remaining terms and substituting back in (2.41) we obtain for the first quantum correction

$$\Gamma_1 = \frac{\mathrm{Vol}(X)}{2}\left[\left(\frac{V_B^{(2)}}{V_B} - \frac{V_A^{(2)}}{V_A}\right)\ln(\sigma)\Bigg|_{\sigma_0}^{\bar{\sigma}-\delta\sigma}\right] + \mathrm{Vol}(X)T_1, \tag{4.70}$$

where we note that once again there only appears one tension term, thus it only adds one extra parameter. Furthermore, we note that the divergence that appeared in the flat FLRW result in (4.26) appears again and we are led once again to impose the condition (4.27). Thus, we finally obtain

$$\Gamma_1 = \mathrm{Vol}(X)T_1. \tag{4.71}$$

which is only a constant. Therefore, the general behaviour is unaltered by the first quantum correction. Carrying out with the analysis to the second quantum correction, we note that for this metric

$$\nabla^2\left(\nabla^2\mathcal{V}\right) = \frac{\gamma}{\sigma^2}V^{(4)} \tag{4.72}$$

$$\left(\nabla\left(\nabla^2\mathcal{V}\right)\right)^2 = \frac{\gamma}{\sigma^2}\left(V^{(3)}\right)^2. \tag{4.73}$$

Therefore, computing the remaining necessary terms we obtain from (2.42) that the second quantum correction term is

$$\begin{aligned}\Gamma_2 = \pm\frac{\mathrm{Vol}(X)i\hbar}{4}\Bigg\{&\frac{V_B^{(4)}}{V_B}H_{KS}(c_B,\sigma)\Bigg|_{\sigma_0}^{\bar{\sigma}} + \left(\frac{V_B^{(3)}}{V_B}\right)^2 I_{KS}(c_B,\sigma)\Bigg|_{\sigma_0}^{\bar{\sigma}} - \frac{V_A^{(4)}}{V_A}H_{KS}(c_A,\sigma)\Bigg|_{\sigma_0}^{\bar{\sigma}}\\ &- \left(\frac{V_A^{(3)}}{V_A}\right)^2 I_{KS}(c_A,\sigma)\Bigg|_{\sigma_0}^{\bar{\sigma}}\Bigg\} + \frac{\mathrm{Vol}(X)\hbar}{\bar{\sigma}}\sqrt{\frac{V_B}{1-c_B\bar{\sigma}}}T_2,\end{aligned} \tag{4.74}$$

where we have defined the functions

$$H_{KS}(c,\sigma) = \int\frac{d\sigma}{\sigma^2\sqrt{4-3c\sigma}} = -\frac{\sqrt{4-3c\sigma}}{4\sigma} - \frac{3c}{8}\left(\frac{\sqrt{4-3c\sigma}}{2}\right), \tag{4.75}$$

$$I_{KS}(c,\sigma) = \int\frac{1-c\sigma}{\sigma^2\left(4-3c\sigma\right)^{3/2}}d\sigma = -\frac{1}{16}\left[\frac{4-c\sigma}{\sigma\sqrt{4-3c\sigma}} + \frac{c}{2}\left(\frac{\sqrt{4-3c\sigma}}{2}\right)\right]. \tag{4.76}$$

Furthermore, we note from this result that the functions H_{KS} and I_{KS} have a divergence if we choose $\sigma_0 = 0$, but this divergence is indpendent of c. Therefore, in order to have a well defined probability we can eliminite those divergences by imposing the conditions

$$\frac{V_B^4}{V_B} = \frac{V_A^4}{V_A}, \qquad \left(\frac{V_B^3}{V_B}\right)^2 = \left(\frac{V_A^3}{V_A}\right)^2. \tag{4.77}$$

We note that as in all the previous cases all the possible tension terms reduce to only one and that it is written in such a way that $\lim_{\bar{\sigma}\to 0}\Gamma_2$ diverges, therefore choosing the appropiate signs the probability of having a universe created at $\bar{\sigma} = 0$ vanishes. However, we note that as in the Bianchi III result we are not avoiding the singularity, we are just preventing this point which has a diferent physical meaning. Furthermore, when we plot the transition probabilities for the semiclassical contribution in (4.67), the first quantum correction in (4.71) and the second quantum correction in (4.74) we obtain the same behavour as the one encountered for the FLRW metric in Figure 4.1.

Chapter 5

Transition probabilities in $f(R)$ gravity

In this chapter, we employ the general framework established for the calculation of vacuum transitions in the presence of gravity, substituting the gravitational sector with modified $f(R)$ gravity. As will be explicitly demonstrated, this modification preserves the quadratic dependence on the momenta within the resulting Hamiltonian constraint, thereby permitting the direct application of the established formalism. We demonstrate that while the general behaviors observed in General Relativity are qualitatively similar to those obtained in $f(R)$ gravity, this modification induces a more rapid decay of the transition probabilities for the majority of models. Consequently, results are presented for FLRW metrics with zero and positive curvature. Specifically, we analyze power-law models of the form $f(R) = R^{1+n}$, exploring the dependence of the transitions on the parameter n, as well as the Starobinsky model defined by $f(R) = R + \beta R^2$.

5.1 Quantum cosmology for FLRW metrics in modified $f(R)$ gravity

To construct the quantum cosmological framework for $f(R)$ gravity coupled to a scalar field, we begin with the total action comprising both gravitational and matter sectors as

$$S = \frac{1}{2}\int d^4x f(R)\sqrt{-g} - \int d^4x\sqrt{-g}\left(\frac{1}{2}g^{\mu\nu}\partial_\mu\phi\partial_\nu\phi + V\right) \tag{5.1}$$

This action generalizes the Einstein-Hilbert formulation by replacing the Ricci scalar R with an arbitrary function $f(R)$, while maintaining the standard kinetic and potential terms for the scalar field ϕ. The coupling between geometry and matter through the metric determinant $\sqrt{-g}$ ensures general covariance of the theory. For the spatially flat FLRW metric in Cartesian coordinates,

$$ds^2 = -N^2(t)dt^2 + a^2(t)(dx^2 + dy^2 + dz^2), \tag{5.2}$$

we compute the essential geometric quantity. The Ricci scalar for this homogeneous and isotropic spacetime takes the form

$$R = 6\left(\frac{\dot{a}^2}{a^2N^2} + \frac{\ddot{a}}{aN^2} - \frac{\dot{a}\dot{N}}{aN^3}\right), \tag{5.3}$$

where the three expected terms respectively represent, the Hubble expansion contribution $(\dot{a}^2/a^2)$, the cosmic acceleration $(\ddot{a}/a)$ and the gauge-dependent term involving the lapse function $(\dot{N})$.

To appropriately address the $f(R)$ term within the action, the methodology established in [98, 103] is adopted. This approach suggests that, in the general scenario, the elimination of the second derivatives of the field a through integration by parts cannot be carried out. The standard procedure for canonical quantization in these circumstances requires the introduction of an extra field, here formally defined as the scalar curvature, R. This is equivalent to the reformulation of the original fourth-order differential equation into a coupled system of two second-order differential equations. Consequently, we can consider (5.3) as a constraint, and by employing the method of Lagrange multipliers, the action can be expressed as

$$\frac{1}{2}\int d^4x\sqrt{-g}f(R) = \frac{1}{2}\int d^4x\left\{Na^3 f(R) - \lambda\left[R - 6\left(\frac{\dot{a}^2}{a^2N^2} + \frac{\ddot{a}}{aN^2} - \frac{\dot{a}\dot{N}}{aN^3}\right)\right]\right\}. \tag{5.4}$$

Here, λ serves as a Lagrange multiplier. The variation of the action with respect to the Ricci scalar R yields

$$\frac{\delta S}{\delta R} = Na^3 f_R(R) - \lambda = 0, \tag{5.5}$$

from which we immediately identify the multiplier as

$$\lambda = Na^3 f_R(R). \tag{5.6}$$

Substituting this back into our constrained action and performing integration by parts on the terms involving time derivatives, we obtain after discarding boundary terms

$$\frac{1}{2}\int d^4x\sqrt{-g}f(R) = \int d^4x\left\{\frac{Na^3}{2}(f - Rf_R) - 3\dot{R}f_{RR}\frac{a^2\dot{a}}{N} - 3f_R\frac{a\dot{a}^2}{N}\right\}. \tag{5.7}$$

where we note that the terms on the right-hand side represent: the potential-like term $(f - Rf_R)$ and the standard kinetic term modified by f_R. For the scalar field sector, assuming homogeneity $(\phi = \phi(t))$, we obtain:

$$\int d^4x\sqrt{-g}\left(\frac{1}{2}g^{\mu\nu}\partial_\mu\phi\partial_\nu\phi + V(\phi)\right) = \int d^4x\left(-\frac{a^3}{2N}\dot{\phi}^2 + Na^3V(\phi)\right). \tag{5.8}$$

Combining both contributions, we arrive at the complete Lagrangian

$$\mathcal{L} = \frac{Na^3}{2}(f - Rf_R) - 3\dot{R}f_{RR}\frac{a^2\dot{a}}{N} - 3f_R\frac{a\dot{a}^2}{N} - \frac{a^3}{2N}\dot{\phi}^2 + Na^3V(\phi). \tag{5.9}$$

This Lagrangian contains all the dynamical information of our system, including both gravitational and matter degrees of freedom. In order to obtain the Hamiltonian constraint, the canonical momenta, defined as $\pi_M = \frac{\partial\mathcal{L}}{\partial\dot{\Phi}^M}$ where $\Phi^M = \{N, a, R, \phi\}$, are computed to be

$$\begin{cases}\pi_N = 0,\\ \pi_a = -3\dot{R}f_{RR}\frac{a^2}{N} - 6f_R\frac{a\dot{a}}{N},\\ \pi_R = -3f_{RR}\frac{a^2\dot{a}}{N},\\ \pi_\phi = \frac{a^3}{N}\dot{\phi}.\end{cases} \tag{5.10}$$

The vanishing of π_N reflects the fact that the lapse function N is a Lagrange multiplier enforcing the Hamiltonian constraint, rather than a dynamical degree of freedom.

Performing the Legendre transformation, we obtain the Hamiltonian constraint

$$H = N\left[-\frac{\pi_a\pi_R}{3f_{RR}a^2} + \frac{1}{3}\frac{f_R}{f_{RR}^2}\frac{\pi_R^2}{a^3} + \frac{\pi_\phi^2}{2a^3} - \frac{a^3}{2}(f - Rf_R) + a^3V(\phi)\right] \approx 0. \tag{5.11}$$

The resulting expression is clearly quadratic in the momenta, consistent with the general restriction specified by the formalism in (1.37). On the other hand, for the case of positive curvature FLRW metric,

$$ds^2 = -N^2(t)dt^2 + a^2(t)\left(dr^2 + \sin^2 r\, d\Omega_2^2\right), \tag{5.12}$$

where $r \in [0, \pi]$ and $d\Omega_2^2$ is the metric on the unit 2-sphere, the geometric quantities become

$$\begin{cases} R = 6\left(\frac{1}{a^2} + \frac{\dot{a}^2}{a^2N^2} + \frac{\ddot{a}}{aN^2} - \frac{\dot{a}\dot{N}}{aN^3}\right), \\ \sqrt{-g} = Na^3 \sin^2 r \sin\theta. \end{cases} \tag{5.13}$$

The additional $1/a^2$ term in the Ricci scalar represents the intrinsic curvature contribution from the spatial sections. Following the same procedure, the Hamiltonian constraint for this case takes the form

$$H = N\left[-\frac{\pi_a\pi_R}{3f_{RR}a^2} + \frac{1}{3}\frac{f_R}{f_{RR}^2}\frac{\pi_R^2}{a^3} + \frac{\pi_\phi^2}{2a^3} - \frac{a^3}{2}(f - Rf_R) + a^3V(\phi) - 3f_R a\right] \approx 0. \tag{5.14}$$

As we can see, the final expresions for Hamiltonian constraints, (5.14) and (5.11), have the general form (1.37) and only differs on the final term $-3f_R a$, in this way we can propose a Hamiltonian constraint that enclose both scenarios as

$$H = N\left[\frac{-\pi_a\pi_R}{3f_{RR}a^2} + \frac{1}{3}\frac{f_R}{f_{RR}^2}\frac{\pi_R^2}{a^3} + \frac{\pi_\phi^2}{2a^3} - \frac{a^3}{2}\left(f - Rf_R\right) + a^3V - 3\kappa a f_R\right] \approx 0. \tag{5.15}$$

where κ stands for the curvature parameter for flat or closed spatial geometries with values $\{0, 1\}$ respectively. This allows identification of the minisuperspace defined by the coordinates $\{\Phi^M\} = \{a, R, \phi\}$, the metric

$$(G^{MN}) = \begin{pmatrix} 0 & -\frac{1}{3f_{RR}a^2} & 0 \\ -\frac{1}{3f_{RR}a^2} & \frac{2}{3}\frac{f_R}{f_{RR}^2a^3} & 0 \\ 0 & 0 & \frac{1}{a^3} \end{pmatrix} \tag{5.16}$$

and the function

$$\mathcal{V} = \frac{a^3}{2}\left[2V - (f - Rf_R)\right] - 3\kappa f_R a. \tag{5.17}$$

which are the starting point for the application of the formalism.

5.2 Transitions for a flat FLRW metric

Having established the Hamiltonian contraint of the model, we now proceed to apply the methodology keeping the model for $f(R)$ arbitrary as far as possible. Our analysis will commence with the spatially flat FLRW metric, which serves as the fundamental geometric background for describing the large-scale structure and evolution of the homogeneous and isotropic universe. Thus from the expression (5.15), taking the case $\kappa = 0$ we obtain the general expressions for the solutions in (2.11) such as

$$C^2(s) = \frac{2\,\mathrm{Vol}(X)^2\left(3Rf - 6RV - 2R^2f_R + 6V^{(1)2}\right)}{3\left(f - 2V - Rf_R\right)}, \tag{5.18}$$

that at the minima of the potential $\phi_{A,B}$, we have $V^{(1)}_{A,B} = 0$, so that

$$C^2(s) = \frac{2\,\mathrm{Vol}^2(X)R\left(3f - 6V_{A,B} - 2Rf_R\right)}{3\left(f - 2V_{A,B} - Rf_R\right)}. \tag{5.19}$$

In order to have the expressions in terms of the scale factor a, the relations between the parameter s and the scalar curvature R are determined by

$$\frac{dR}{ds} = \frac{(-f + Rf_R + 2V)(-3f + 6V + Rf_R)}{2\,\mathrm{Vol}(X) f_{RR}\left(-3Rf + 6RV + 2R^2 f_R - 6V^{(1)2}\right)}. \tag{5.20}$$

$$\frac{da}{ds} = \frac{a\,(f - 2V_{A,B} - Rf_R)}{2\,\mathrm{Vol}^2(X)\left(3f - 6V_{A,B} - 2Rf_R + 6V^{(1)2}\right)}, \tag{5.21}$$

$$\frac{da}{dR} = \frac{aRf_{RR}}{(-3f + 6V + Rf_R)}. \tag{5.22}$$

Thus, the semiclassical contribution to the transition probability in (2.32), when evaluated for the spatially flat FLRW metric, takes the general form for an arbitrary $f(R)$ gravity model as follows

$$\begin{aligned}
\Gamma_0 = \mp \frac{\sqrt{6}\,\mathrm{Vol}(X) i}{\hbar} & \left\{ \int_{a_0}^{\bar{a}-\delta a} a^2 \sqrt{\frac{-f + 2V_B + Rf_R}{R\,(-3f + 6V_B + 2Rf_R)}}\,(-3f + 6V_B + 2Rf_R)\,da \right. \\
& \left. - \int_{a_0}^{\bar{a}-\delta a} a^2 \sqrt{\frac{-f + 2V_A + Rf_R}{R\,(-3f + 6V_A + 2Rf_R)}}\,(-3f + 6V_A + 2Rf_R)\,da \right) \\
& + \frac{\mathrm{Vol}(X)}{\hbar} a^3 T_0 + \frac{2\,\mathrm{Vol}(X) i}{\hbar} \int_{\bar{s}-\delta s}^{\bar{s}+\delta s} \frac{ds}{C(s)} \left[\frac{a^3}{2}\,(f - Rf_R) - \left.\frac{a^3}{2}\,(f - Rf_R)\right|_{\phi=\phi_A} \right],
\end{aligned} \tag{5.23}$$

where by virtue of (5.22), it is evident that R is functionally dependent upon the scale factor a and the potential $V(\phi)$; that is, $R = R(a, V)$. Consequently, the term associated with $f(R)$ must be retained until its explicit functional form is determined for each specific $f(R)$ function. Furthermore, based on the structure of the initial term within the integral, which involves a non constant potential, it is posible to define a tension term T_0. This term is demonstrably identical to that obtained in the framework of the Einstein-Hilbert action (See chapter 4). Additionally, an extra tension term associated with $f(R)$ emerges in the third line. Whether this extra term is additive to T_0 is conditional upon the specific form of the function $f(R)$ and the derived relationships between the metric variables and R. On the other hand, for the first quantum correction, we find

$$\nabla^2 \mathcal{V} = V^{(2)} - R + \frac{f_R\,(f_{RR} + Rf_{RRR})}{3f_{RR}^2} \tag{5.24}$$

therefore, using (2.33), we have for the first correction

$$\begin{aligned}
\Gamma_1 = \mathrm{Vol}(X) & \left\{ \int_{a_0}^{\bar{a}-\delta a} \frac{\left[3f_{RR}^2\left(V_B^{(2)} - R\right) + f_R\,(f_{RR} + Rf_{RRR})\right]}{aRf_{RR}^2} da \right. \\
& \left. - \int_{a_0}^{\bar{a}-\delta a} \frac{\left[3f_{RR}^2\left(V_A^{(2)} - R\right) + f_R\,(f_{RR} + Rf_{RRR})\right]}{aRf_{RR}^2} da \right\} \\
& + \frac{\mathrm{Vol}(X)}{2} T_1 \\
& + \mathrm{Vol}^2(X) \int_{\bar{s}-\delta s}^{\bar{s}+\delta s} \frac{ds}{C^2(s)} \left[\frac{f_R\,(f_{RR} + Rf_{RRR})}{3f_{RR}^2} - R \right. \\
& \left. - \left.\frac{f_R\,(f_{RR} + Rf_{RRR})}{3f_{RR}^2}\right|_{\phi=\phi_A} + \left.R\right|_{\phi=\phi_A} \right].
\end{aligned} \tag{5.25}$$

Now, in the same way as with the semiclassical contribution, we can divide the integral where the field is not constant and be left with two tension terms, one that is associated to the General Relativity case, T_1, and another associated with the function $f(R)$ and its derivatives. Finally, for the second correction we have

$$\begin{aligned}\nabla^2\left(\nabla^2\mathcal{V}\right) =&\frac{2f_R}{9a^3f_{RR}^4}\left[-3Rf_{RRR}^2+f_{RR}\left(f_{RRR}+2Rf_{RRRR}\right)\right]+\frac{V^{(4)}}{a^3}\\&+\frac{2f_R^2}{9a^3f_{RR}^6}\left[6Rf_{RRR}^2-2f_{RR}f_{RRR}\left(f_{RRR}+3Rf_{RRRR}\right)\right.\\&\left.+f_{RR}^2\left(f_{RRRR}+Rf_{RRRRR}\right)\right]\end{aligned}\tag{5.26}$$

and

$$\begin{aligned}\left[\nabla\left(\nabla^2\mathcal{V}\right)\right]^2 =&\frac{2f_R}{27a^3f_{RR}^4}\left(-2f_{RR}+Rf_{RRR}\right)^2+\frac{V^{(3)2}}{a^3}\\&+\frac{4Rf_R^2}{27a^3f_{RR}^6}\left(-2f_{RR}+Rf_{RRR}\right)\left(-2f_{RRR}^2+f_{RR}f_{RRRR}\right)\\&+\frac{2R^2f_R^3}{27a^3f_{RR}^8}\left(-2f_{RRR}^2+f_{RR}f_{RRRR}\right)^2.\end{aligned}\tag{5.27}$$

Then, the expression for Γ_2 becomes

$$\begin{aligned}\Gamma_2 = \frac{i\hbar\,\mathrm{Vol}(X)}{2}&\left\{\int_{a_0}^{\bar{a}-\delta a}\frac{\left(9f_{RR}^6V_B^{(4)}+U\right)}{\sqrt{6}a^4Rf_{RR}^6}\sqrt{\frac{-f+2V_B+Rf_R}{R\left(-3f+6V_B+2Rf_R\right)}}\right.\\&+\int_{a_0}^{\bar{a}-\delta a}\frac{\left(27f_{RR}^8V_B^{(3)2}+W\right)}{2\sqrt{6}a^4Rf_{RR}^8}\left[\frac{-f+2V_B+Rf_R}{R\left(-3f+6V_B+2Rf_R\right)}\right]^{3/2}\\&-\int_{a_0}^{\bar{a}-\delta a}\frac{\left(9f_{RR}^6V_A^{(4)}+U\right)}{\sqrt{6}a^4Rf_{RR}^6}\sqrt{\frac{-f+2V_A+Rf_R}{R\left(-3f+6V_A+2Rf_R\right)}}\\&\left.-\int_{a_0}^{\bar{a}-\delta a}\frac{\left(27f_{RR}^8V_A^{(3)2}+W\right)}{2\sqrt{6}a^4Rf_{RR}^8}\left[\frac{-f+2V_A+Rf_R}{R\left(-3f+6V_A+2Rf_A\right)}\right]^{3/2}\right\}\\&+\frac{\hbar\,\mathrm{Vol}(X)}{\bar{a}^3}T_2\\&+\frac{i\hbar}{2}\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{\mathrm{Vol}^3(X)ds}{C^3(s)}\left(\frac{1}{9a^3}\right)\left(\frac{U}{f_{RR}^6}-\frac{U}{f_{RR}^6}\,|_{\phi=\phi_A}\right)\\&+\frac{i\hbar}{2}\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{\mathrm{Vol}^5(X)ds}{C^5(s)}\left(\frac{1}{27a^3}\right)\left(\frac{W}{f_{RR}^8}-\frac{W}{f_{RR}^8}\,|_{\phi=\phi_A}\right)\end{aligned}\tag{5.28}$$

where were defined

$$\begin{aligned}U = 2f_R&\left\{f_{RR}^2\left[f_R(f_{RRRR}+f_{RRRRR}R)-3f_{RRR}^2R\right]\right.\\&\left.-2f_Rf_{RR}f_{RRR}(f_{RRR}+3f_{RRRR}R)+6f_Rf_{RRR}^3R+f_{RR}^3(f_{RRR}+2f_{RRRR}R)\right\},\end{aligned}\tag{5.29}$$

$$\begin{aligned}W =& 2f_Rf_{RR}^4\left(-2f_{RR}+Rf_{RRR}\right)^2\\&+4Rf_R^2f_{RR}^2\left(-2f_{RR}+Rf_{RRR}\right)\left(-2f_{RRR}^2+f_{RR}f_{RRRR}\right)\\&+2R^2f_R^3\left(-2f_{RRR}^2+f_{RR}f_{RRRR}\right)^2,\end{aligned}\tag{5.30}$$

and a tension term T_2. From the expressions for Γ_0, Γ_1 and Γ_2 we can see that the tension terms obtained in General Relativity are preserved identically but new contributions are added that will depend on the modified gravity model.

5.2.1 Constant Ricci Scalar Scenario

For this section, we can see, that a possible solution in the expresion (5.20) is to consider an approach where the Ricci scalar is constant (i.e., $dR = 0$). This consideration, although restrictive, allows us to simplify the probability calculations. Additionally, in the Euclidean treatment for modified gravity, in [105] a formalism is develop for computing the Euclidean action and bounce solution, extending the Coleman-De Luccia (CDL) analysis to gravity $f(R)$ using the thin-wall approximation, in this work the consideration of constant Ricci scalar configurations in $f(R)$ gravity theories implies that in maximally symmetric spacetime regions, such as false and true vacuum states in decay processes, the Ricci scalar naturally assumes constant values that characterize these configurations. This constant value not only simplifies mathematical analysis through algebraic equations rather than differential equations, but also ensures regularity of the bounce solutions describing new vacuum bubble formation. In this manner, it is consistent to consider the sole condition under which $dR = 0$ holds without imposing $da = 0$ in the expresion (5.20) and (5.22), that is

$$-3f + 6V + Rf_R = 0. \tag{5.31}$$

On the other hand, we have that the Hubble parameter is $H = \frac{\dot{a}}{a}$, and since we have the freedom to choose the lapse function, choosing $N = 1$, it follows that for the flat FLRW metric

$$R = 6\left[2H^2 + \dot{H}\right]. \tag{5.32}$$

However, if we are interested in having an constant Ricci scalar, we need the Hubble parameter H, to be constant as well, in this way, $\dot{R} = 0$, and then the expression

$$6V + Rf_R - 3f|_{R=12H^2} = 0 \tag{5.33}$$

is satisfied. Nevertheless, we cannot take this expression and look for a unique solution for f that satisfies it, because the restriction on R has already been made, so the solution to the differential equation is not the only one for f. What has been found is an algebraic equation whose solution will give us the constant Hubble parameter given a particular form of the function f and the relationship between R and a is completely determined. In general, for arbitrary $f(R)$ models, this relationship implies that the Ricci scalar is a function of the potential and parameters of the model, that in the constant field regions, they are purely constant. Consequently, the semiclassical contribution (5.23) can be rewrite as

$$\begin{aligned}\Gamma_0 = &\mp \frac{\mathrm{Vol}(X)}{\hbar} i \left[L\left(V_B\right) - L\left(V_A\right)\right] a^3\Big|_{a_0}^{\bar{a}-\delta_0} + \frac{\mathrm{Vol}(X)}{\hbar}\bar{a}^3 T_0 \\ &+ \frac{2\,\mathrm{Vol}(X) i}{\hbar}\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{ds}{C(s)}\left[\frac{a^3}{2}\left(f - Rf_R\right) - \frac{a^3}{2}\left(f - Rf_R\right)\Big|_{\phi=\phi_A}\right]\end{aligned} \tag{5.34}$$

with

$$L\left(V_{A,B}, f(R), f_R\right) = \sqrt{\frac{2}{3}}\sqrt{\frac{-f + Rf_R + 2V}{R(-3f + 2Rf_R + 6V)}}(-3f + 2Rf_R + 6V). \tag{5.35}$$

This expression allows to consider as initial value $a_0 = 0$, in order to access to the singularity. In the same way, for the first quantum correction we define

$$M\left(V_{A,B}\right) = \frac{3f_{RR}^2\left(V_{A,B}^{(2)} - R\right) + f_R\left(f_{RR} + Rf_{RRR}\right)}{Rf_{RR}^2}\;|_{\phi=\phi_A,\phi_B}\,, \tag{5.36}$$

so we can rewrite

$$\begin{aligned}\Gamma_1 =& \mathrm{Vol}(X)\left\{\left[M\left(V_B\right)-M\left(V_A\right)\right]\ln(a)|_{a_0}^{\bar{a}-\delta a}\right\}+\frac{\mathrm{Vol}(X)}{2}T_1\\ &+\mathrm{Vol}^2(X)\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{ds}{C^2(s)}\left[\frac{f_R\left(f_{RR}+Rf_{RRR}\right)}{3f_{RR}^2}-R\right.\\ &\left.-\left.\frac{f_R\left(f_{RR}+Rf_{RRR}\right)}{3f_{RR}^2}\right|_{\phi=\phi_A}+R|_{\phi=\phi_A}\right],\end{aligned} \tag{5.37}$$

as we can see the first quantum correction term becomes ill-defined when considering the initial condition $a_0 = 0$. However, to ensure well defined contribution we impose the matching condition $M(V_A) = M(V_B)$, which give conditions on the potential in the false and true vacuum regions. In this way we have

$$\begin{aligned}\Gamma_1 =&\frac{\mathrm{Vol}(X)}{2}T_1\\ &+\mathrm{Vol}^2(X)\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{ds}{C^2(s)}\left[\frac{f_R\left(f_{RR}+Rf_{RRR}\right)}{3f_{RR}^2}-R\right.\\ &\left.-\left.\frac{f_R\left(f_{RR}+Rf_{RRR}\right)}{3f_{RR}^2}\right|_{\phi=\phi_A}+R|_{\phi=\phi_A}\right],\end{aligned} \tag{5.38}$$

and

$$\begin{aligned}&\frac{3f_{RR}^2\left(V_A^{(2)}-R\right)+f_R\left(f_{RR}+Rf_{RRR}\right)}{Rf_{RR}^2}\ |_{\phi=\phi_A}=\\ &\qquad=\frac{3f_{RR}^2\left(V_B^{(2)}-R\right)+f_R\left(f_{RR}+Rf_{RRR}\right)}{Rf_{RR}^2}\ |_{\phi=\phi_B}.\end{aligned} \tag{5.39}$$

Let's remark that given the dependency of $R = R(V)$ and some model parameters, said expression is only a condition on the potential and its derivatives. In the same way, for the second quantum correction we can define

$$Q(V_{A,B},V_{A,B}^{(n)})=\frac{\left(9f_{RR}^6V_{A,B}^{(4)}+U\right)}{\sqrt{6}Rf_{RR}^6}\sqrt{\frac{-f+2V_{A,B}+Rf_R}{R\left(-3f+6V_{A,B}+2Rf_R\right)}}\ |_{\phi=\phi_A,\phi_B} \tag{5.40}$$

and

$$S(V_{A,B},V_{A,B}^{(n)})=\frac{\left(27f_{RR}^8V_{A,B}^{(3)2}+W\right)}{2\sqrt{6}Rf_{RR}^8}\left[\frac{-f+2V_{A,B}+Rf_R}{R\left(-3f+6V_{A,B}+2Rf_R\right)}\right]^{3/2}\ |_{\phi=\phi_A,\phi_B}. \tag{5.41}$$

Such that the expression for the second quantum correction in (5.28) can be written as

$$\begin{aligned}\Gamma_2 =\pm&\frac{i\hbar\,\mathrm{Vol}(X)}{2}\{\left[Q\ |_{\phi=\phi_B}-Q\ |_{\phi=\phi_A}\right]\left.\left(\frac{1}{3a^3}\right)\right|_{a_0}^{\bar{a}-\delta a}\\ &+\left[S\ |_{\phi=\phi_B}-S\ |_{\phi=\phi_A}\right]\left.\left(\frac{1}{3a^3}\right)\right|_{a_0}^{\bar{a}-\delta d}\Bigg\}\\ &+\frac{\hbar\,\mathrm{Vol}(X)}{\bar{a}^3}T_2\\ &+\frac{i\hbar}{2}\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{\mathrm{Vol}^3(X)ds}{C^3(s)}\left(\frac{1}{9a^3}\right)\left(\frac{U}{f_{RR}^6}-\frac{U}{f_{RR}^6}\ |_{\phi=\phi_A}\right)\\ &+\frac{i\hbar}{2}\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{\mathrm{Vol}^5(X)ds}{C^5(s)}\left(\frac{1}{27a^3}\right)\left(\frac{W}{f_{RR}^8}-\frac{W}{f_{RR}^8}\ |_{\phi=\phi_A}\right).\end{aligned} \tag{5.42}$$

Analogous to the assumptions for the first quantum correction, to implement the condition $a_0 = 0$, we need to impose the constraints

$$Q_A = Q_B, \quad S_A = S_B, \tag{5.43}$$

Under these conditions, the expression for the amplitude reduces to

$$\begin{aligned}\Gamma_2 = &+ \frac{\hbar\,\mathrm{Vol}(X)}{\bar{a}^3} T_2 \\ &+ \frac{i\hbar}{2}\int_{\bar{s}-\delta s}^{\bar{s}+\delta s} \frac{\mathrm{Vol}^3(X)ds}{C^3(s)}\left(\frac{1}{9a^3}\right)\left(\frac{U}{f_{RR}^6} - \frac{U}{f_{RR}^6}\,|_{\phi=\phi_A}\right) \\ &+ \frac{i\hbar}{2}\int_{\bar{s}-\delta s}^{\bar{s}+\delta s} \frac{\mathrm{Vol}^5(X)ds}{C^5(s)}\left(\frac{1}{27a^3}\right)\left(\frac{W}{f_{RR}^8} - \frac{W}{f_{RR}^8}\,|_{\phi=\phi_A}\right).\end{aligned} \tag{5.44}$$

As we can notice from the preceding expressions, the primary objective is to determine the tension contributions arising from the $f(R)$ modifications associated with each correction term. It is also pertinent to note that within the framework of General Relativity [161], accessing the singularity demands the imposition of specific conditions upon the potential function and its derivatives at the minima, albeit this requirement is generally less complicated than that required for $f(R)$. The conditions obtained in (5.39) and (5.43), are equivalent to those for General Relativity.

5.2.2 $f(R) = R^{1+n}$

As our initial case study, we examine the power-law $f(R)$ gravity model given by $f(R) = R^{1+n}$, focusing on addopting the condition of the constant Ricci scalar. This model represents a particularly interesting generalization of Einstein gravity introducing non trivial modifications to the gravitational dynamics (see or example [177–180]). So, let us consider the expresion (5.33) and solve for the Hubble parameter H, such that

$$f(R) = R^{(1+n)} \Rightarrow H = \sqrt{\frac{6^{\frac{1}{1+n}}\left(\frac{2-n}{V}\right)^{-\frac{1}{1+n}}}{12}} \tag{5.45}$$

in this way, from the simplified expression in (5.34), we can write for the semiclassical contribution

$$\begin{aligned}\Gamma_0 = &\mp \frac{\mathrm{Vol}(X)}{\hbar} i\left[L\left(V_B\right) - L\left(V_A\right)\right]\bar{a}^3 + \frac{\mathrm{Vol}(X)}{\hbar}\bar{a}^3 T_0 \\ &- \frac{\mathrm{Vol}(X)i}{\hbar}\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{ds}{C(s)}a^3\left[n\left(\frac{3V}{-n+2}\right) - n\left(\frac{3V_A}{-n+2}\right)\right],\end{aligned} \tag{5.46}$$

where

$$\begin{aligned}L(V_{A,B}) = &\left\{(2n-1)\left[6^{\frac{1}{n+1}}\left(\frac{2-n}{V}\right)^{-\frac{1}{n+1}}\right]^{n+1} + 6V\right\}\times \\ &\times\sqrt{\frac{2n\left[6^{\frac{1}{n+1}}\left(\frac{2-n}{V}\right)^{-\frac{1}{n+1}}\right]^{n+1} + 4V}{2^{\frac{n+2}{n+1}}3^{\frac{2n+3}{n+1}}V\left(\frac{2-n}{V}\right)^{-\frac{1}{n+1}} + (6n-3)\left[6^{\frac{1}{n+1}}\left(\frac{2-n}{V}\right)^{-\frac{1}{n+1}}\right]^{n+2}}}.\end{aligned} \tag{5.47}$$

As we can see, the last term in the expression (5.46), allows us to fullfill the condition of separability (2.43), so we can defined an adittional tension term. But it has the same dependence on the potential V as the tension term T_0, and is multiplied by the same power of the scale factor. It only differs by a constant that depends on the parameter n of the model, so we can define a single tension term. Thus, Γ_0 can be expressed as

$$\Gamma_0 = \mp\frac{\mathrm{Vol}(X)}{\hbar} i\left[L\left(V_B\right) - L\left(V_A\right)\right]\bar{a}^3 + \frac{\mathrm{Vol}(X)}{\hbar}\bar{a}^3\left[1 + \left(\frac{3n}{2-n}\right)\right]T_0 \tag{5.48}$$

Expression (5.48) shows that the semiclassical contribution includes an additional correction in the tension term, arising from $f(R)$. This new term induces a sign change in the vicinity of $n = 2$. Notably, in the limit where $n \to 0$, this expression recovers the standard result for the semiclassical contribution from general relativity, at the opposite end, $n \to \infty$, the term accompanying the tension converges to -2, remaining finite. To grasp how transition probabilities behave, it is essential to determine the value ranges for V and n that ensure a well behaved probability. Additionally, we must identify the correct combination of signs where ambiguity arises, as suggested by the formalism. First, given $V > 0$, there are two scenarios to consider based on the value of n.

- For $0 < n < 2$, the function L does not contribute to the expression. Consequently, the choice of sign in Eq. (5.48) is irrelevant.
- For $n > 2$, the function L does contribute. In this regime, the negative sign in Eq. (5.48) must be chosen to ensure the probability is well defined.

So for a general selection we keep the negative sign. For the sign concerning to (2.39), we need to choose a positive sign. Even with the change of sign in the tension terms, causing the probability to increase, it remains bounded even as n approaches infinity. Conversely, if $V < 0$, we need to choose a positive/negative sign in the exponential for the regions $0 < n < 2$ and $n > 2$, respectively, and consider the negative sign in (5.48), for a well behaved probability for $n > 0/\{2\}$. Additionally, in the limit $n \to \infty$ we have

$$\Gamma_0 = a^3 \frac{\mathrm{Vol}(X)}{\hbar} \left[\pm 4i(V_A - V_B) - 2T_0\right] \tag{5.49}$$

which only have the tension term as contribution to the probability. Now, to depict the overall behavior of probability considering different values of n, in Figure 5.1 we present the semiclassical contribution, specifically considering the scenario for positive potentials and choosing the conditions $V_B = 5$, $V_A = 10$ and $T_0 = 1$. As illustrated in the figure, for $0 < n < 2$ the probability decreases

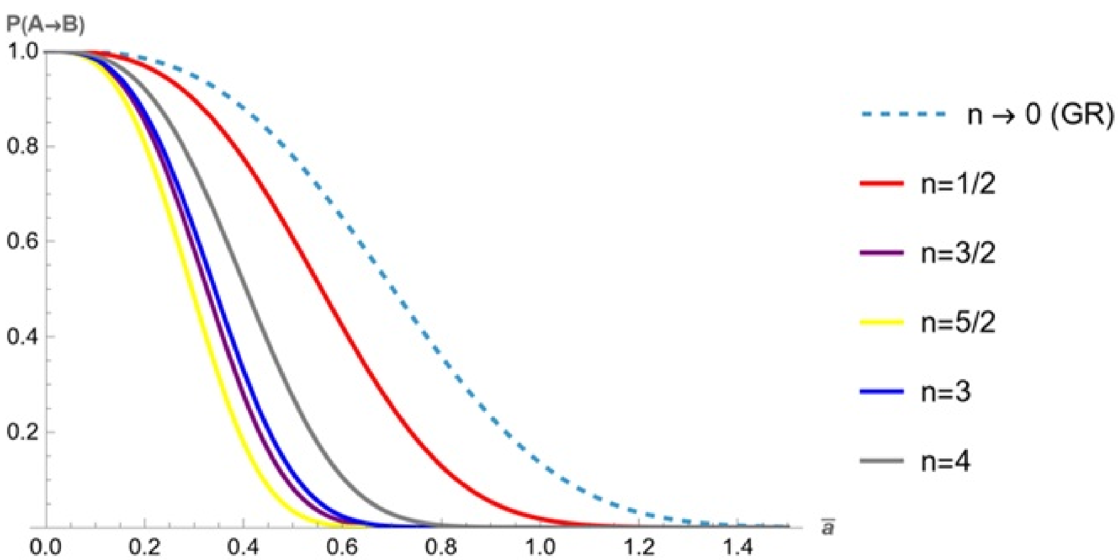

Figure 5.1: Semiclassical contribution for $f(R) = R^{1+n}$ for different values of n. $n \to 0$ (Dashed line), $n = 1/2$ (Red line), $n = 3/2$ (Purple line), $n = 5/2$ (Yellow line), $n = 3$ (Blue line), $n = 4$ (Gray line). With the parameters $V_B = 5$, $V_A = 10$ and $T_0 = 1$.

faster as we approach $n = 2$. However, for $n > 2$, where the change of sign in the tensions occurs, the probability decays slower as the scale factor increases. Moving forward with the first quantum correction, we found

$$\nabla^2\mathcal{V} = V^{(2)} - 2^{\frac{n+2}{n+1}}3^{-\frac{n}{n+1}}\left(\frac{2-n}{V}\right)^{-\frac{1}{n+1}}, \tag{5.50}$$

that leads us to

$$\begin{aligned}\Gamma_1 &= \frac{\mathrm{Vol}(X)}{2}\left[M\left(V_B\right) - M\left(V_A\right)\right]\ln(a)\Big|_{a_0}^{\bar{a}-\delta a} \\ &+ \frac{\mathrm{Vol}(X)}{2}T_1 \\ &- \mathrm{Vol}^2(X)\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{ds}{C^2(s)}\left(\frac{2^{2+n}}{3^n}\right)^{\frac{1}{1+n}}\left(\frac{1}{2-n}\right)^{\frac{1}{1+n}}\left(V^{\frac{1}{1+n}} - V_A^{\frac{1}{1+n}}\right)\end{aligned} \tag{5.51}$$

where, we need to impose $M(V_B) = M(V_A)$, that implies

$$V_B^{(2)}\left(-\frac{V_B}{n-2}\right)^{-\frac{1}{n+1}} = V_A^{(2)}\left(-\frac{V_A}{n-2}\right)^{-\frac{1}{n+1}}, \tag{5.52}$$

in order to be able to consider $a_0 = 0$. It must be noted that in the limit $n \to 0$, the condition imposed upon the potential and its derivatives is precisely that which is obtained for the case corresponding to General Relativity. In this manner, we are left with

$$\Gamma_1 = \frac{\mathrm{Vol}(X)}{2}T_1 + \mathrm{Vol}(X)\left(\frac{2^{2+n}}{3^n}\right)^{\frac{1}{1+n}}\left(\frac{1}{2-n}\right)^{\frac{1}{1+n}}T_1^{f(R)}, \tag{5.53}$$

where, analogously to the semiclassical contribution, an additional tension term associated with $f(R)$ has been defined. This expression reveals two key features, a constant term that reduces the probability from its maximum value of 1, and another n-dependent contribution whose behavior changes around the critical point $n = 2$. Furthermore, the expression remains finite in the limit $n \to \infty$, giving

$$\lim_{n\to\infty}\mathrm{Vol}(X)\left(\frac{2^{2+n}}{3^n}\right)^{\frac{1}{1+n}}\left(\frac{1}{2-n}\right)^{\frac{1}{1+n}}T_1^{f(R)} = \frac{2}{3}\,\mathrm{Vol}(X)T_1^{f(R)}. \tag{5.54}$$

In this manner, Figure 5.2 shows the sum of the semiclassical contribution and the first quantum correction, considering positive potentials using the parameter values $V_B = 5$, $V_A = 10$, $T_0 = 1$, $T_1 = 0.1$, and $T_1^{f(R)} = 0.05$. We can see that the maximum value of the probability is lower in the range $0 < n < 2$ than it is for $n > 2$, but both below 1. This effect is attributed to a sign change in the term derived from $f(R)$. Now, finally, for the second quantum correction, we have

$$\nabla^2\left(\nabla^2\mathcal{V}\right) = \frac{V^{(4)}}{a^3} \tag{5.55}$$

and

$$\left[\nabla\left(\nabla^2\mathcal{V}\right)\right]^2 = \frac{\left(V^{(3)}\right)^2}{a^3} + \frac{8\left[6^{\frac{1}{n+1}}\left(\frac{2-n}{V}\right)^{-\frac{1}{n+1}}\right]^{2-n}}{27a^3n^2(n+1)}, \tag{5.56}$$

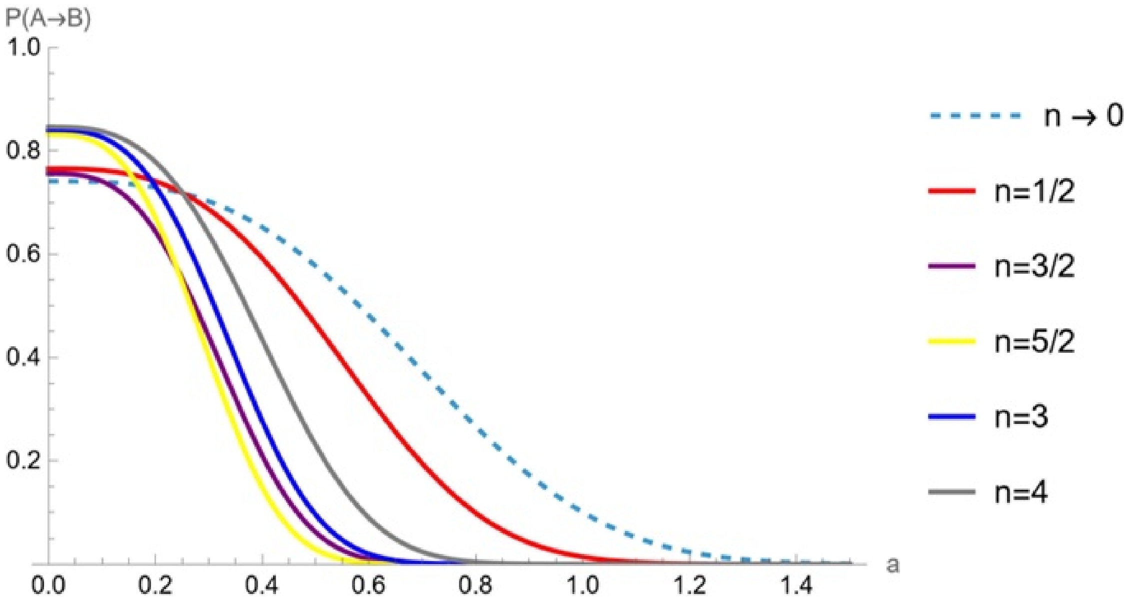

Figure 5.2: First Quantum Correction $\Gamma_0 + \Gamma_1$ for $f(R) = R^{1+n}$ ussing different values of n. $n \to 0$ (Dashed line), $n = 1/2$ (Red line), $n = 3/2$ (Purple line), $n = 5/2$ (Yellow line), $n = 3$ (Blue line)m and $n = 4$ (Gray line). With the parameters $V_B = 5$, $V_A = 10$, $T_0 = 1$, $T_1 = 0.1$, and $T_1^{f(R)} = 0.05$.

in this way, applying the expression found for the second correction in (5.44), we obtain the following expression

$$\begin{aligned}\Gamma_2 = &\pm \frac{i\hbar\,\mathrm{Vol}(X)}{2}\left\{\left[Q\left(V_B\right)+S\left(V_B\right)-Q\left(V_A\right)-S\left(V_A\right)\right]\left(\frac{1}{3a^3}\right)\Bigg|_{a_0}^{\bar{a}-\delta_0}\right\}\\ &+\frac{\hbar\,\mathrm{Vol}(X)}{a^3}T_2+\\ &+\frac{i\hbar}{2}\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{\mathrm{Vol}^5(X)ds}{C^5(s)}\left(\frac{1}{a^3}\right)\left(\frac{8\left[\left(-\frac{6V}{n-2}\right)^{\frac{1}{n+1}}\right]^{2-n}}{27n^2(n+1)}-\frac{8\left[\left(-\frac{6V_A}{n-2}\right)^{\frac{1}{n+1}}\right]^{2-n}}{27n^2(n+1)}\right),\end{aligned} \tag{5.57}$$

where

$$\begin{aligned}Q(V_{A,B}) =&2^{-\frac{n+3}{2n+2}}3^{\frac{3n+1}{2n+2}}V_{A,B}^{(4)}\left(-\frac{V_{A,B}}{n-2}\right)^{-\frac{1}{n+1}}\times\\ &\times\sqrt{\frac{\left[n\left(6^{\frac{1}{n+1}}\left(-\frac{V_{A,B}}{n-2}\right)^{\frac{1}{n+1}}\right)^{n+1}+2V_{A,B}\right]}{6^{\frac{n+2}{n+1}}V_{A,B}\left(-\frac{V_{A,B}}{n-2}\right)^{\frac{1}{n+1}}+(2n-1)\left[6^{\frac{1}{n+1}}\left(-\frac{V_{A,B}}{n-2}\right)^{\frac{1}{n+1}}\right]^{n+2}}}\end{aligned} \tag{5.58}$$

and

$$
\begin{aligned}
S(V_{A,B}) =& \frac{\left\{27n^2(n+1)\left(V_{A,B}^{(3)}\right)^2\left[6^{\frac{1}{n+1}}\left(-\frac{V_{A,B}}{n-2}\right)^{\frac{1}{n+1}}\right]^n + 2^{\frac{3n+5}{n+1}}9^{\frac{1}{n+1}}\left(-\frac{V_{A,B}}{n-2}\right)^{\frac{2}{n+1}}\right\}}{2\sqrt{6}a^4n^2(n+1)}\times \\
&\times\left\{\frac{n\left[6^{\frac{1}{n+1}}\left(-\frac{V_{A,B}}{n-2}\right)^{\frac{1}{n+1}}\right]^{n+1}+2V_{A,B}}{6^{\frac{n+2}{n+1}}V\left(-\frac{V_{A,B}}{n-2}\right)^{\frac{1}{n+1}}+(2n-1)\left[6^{\frac{1}{n+1}}\left(-\frac{V_{A,B}}{n-2}\right)^{\frac{1}{n+1}}\right]^{n+2}}\right\}^{3/2}\times \\
&\times\left[6^{\frac{1}{n+1}}\left(-\frac{V_{A,B}}{n-2}\right)^{\frac{1}{n+1}}\right]^{-n-1}.
\end{aligned}
\tag{5.59}
$$

Similar to the first quantum correction, we encounter an indeterminacy in the constant field region when approaching the initial singularity at $a_0 = 0$. To resolve this and properly define the quantum transition amplitude in this limit, we impose the matching condition $Q_A + S_A = Q_B + S_B$. This condition imposes that the terms of tension govern. Also, an additional tension term that accounts for the modified gravity contributions can be defined. After implementing these considerations, we obtain the following expression for the second quantum correction

$$
\Gamma_2 = \frac{\hbar\,\mathrm{Vol}(X)}{\bar{a}^3}T_2 + \frac{\hbar\,\mathrm{Vol}(X)}{\bar{a}^3}\frac{8\left[\frac{-6}{(n-2)}\right]^{\frac{2-n}{n+1}}}{27n^2(n+1)}T_2^{f(R)}. \tag{5.60}
$$

Of particular significance is the second quantum correction of modified gravity term $T_2^{f(R)}$, which exhibits a highly non trivial dependence on the power-law exponent n. Unlike the semiclassical and first contributions, this term does not admit a well defined $n \to 0$ limit that would recover the corresponding General Relativity results, indicating fundamentally new conditions in the high-curvature regime of our $f(R)$ gravity model. Now, to assess the influence of the tension terms, Figure 5.3 presents the transition probability incorporating the second quantum correction. The calculation was performed considering the following set of physical parameters: $V_B = 5$, $V_A = 10$, $T_0 = 1$, $T_1 = 0.1$, $T_1^{f(R)} = 0.05$, $T_2 = 5\times10^{-4}$, and $T_2^{f(R)} = 10^{-4}$. The graph reveals that the quantum transition probabilities exhibit a non singular behavior that systematically avoids the initial singularity. The probability distribution reaches a finite maximum value, therefore, the second order quantum correction implies that the most probable size of the universe to be created is at a finite non zero value of the scale factor. Respect the n parameter, behaves in such a way that as approaches to zero, the transition probability decreases due to the divergent behavior of the ($f(R)$ dependent tension term. It is observed that the maximum value of the transition probability increases as the parameter n does; nevertheless, this probability remains bounded, as the tension term associated with $f(R)$ asymptotically approaches zero in the limit $n \to \infty$. We want to emphasize that the n dependent coefficient multiplying the modified gravity tension term $T_2^{f(R)}$ shows distinct behavior across different intervals. Specifically, when n lies in the interval $(0, 2)$, this coefficient acquires real values throughout the entire range and for all values $n > 2$, the coefficient becomes complex and vanishes as $n \to \infty$.

5.2.3 Models with R^2 terms

In this section we will review a particular case of the power-law modification $f(R) = R^{1+n}$. Additionally, we include the Starobinsky model (See [98, 181]) $f(R) = R + \beta R^2$. For this, we consider the condition given in (5.33) and solve the Hubble parameter in the aforementioned

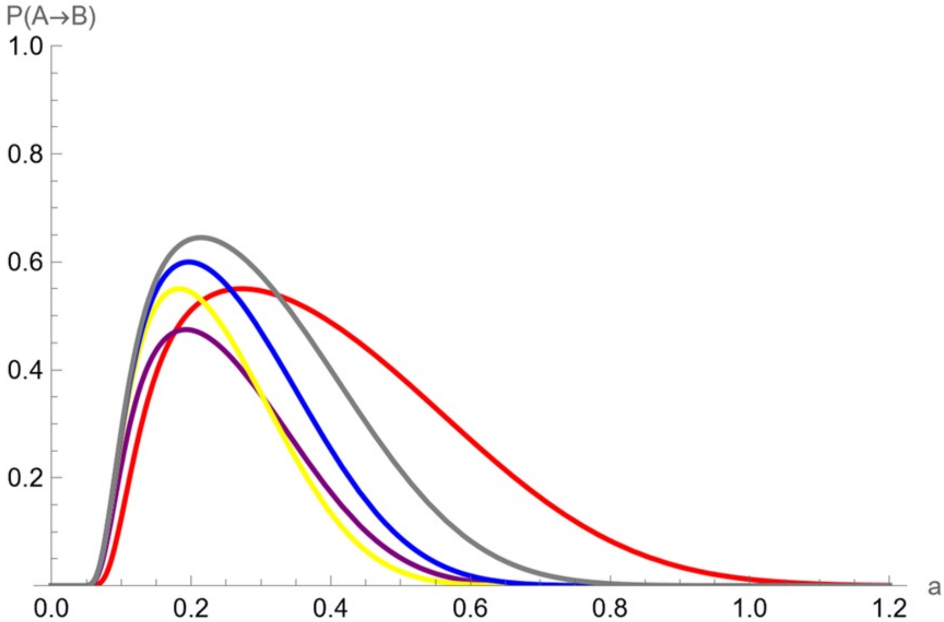

Figure 5.3: Second Quantum Correction $\Gamma_0 + \Gamma_1 + \Gamma_2$ for $f(R) = R^{1+n}$ using different values of n. $n = 0.05$ (Dashed line), $n = 1/2$ (Red line), $n = 3/2$ (Purple line), $n = 5/2$ (Yellow line), $n = 3$ (Blue line), $n = 4$ (Gray line) and $n \to \infty$ (Dotted line). With the parameters $V_B = 5$, $V_A = 10$, $\epsilon = 1$, $T_0 = 1$, $T_0^{f(R)} = 1$, $T_1 = 0.1$, $T_1^{f(R)} = 0.05$, $T_2 = 10^{-3}$, and $T_2^{f(R)} = 10^{-5}$.

models. This yields the following expressions

$$\begin{aligned} f(R) = R^2 &\Rightarrow H = \left(\frac{\sqrt{6V}}{12}\right)^{\frac{1}{2}}, \\ f(R) = R + \beta R^2 &\Rightarrow H = \sqrt{\frac{\sqrt{1+6V\beta}-1}{12\beta}}. \end{aligned} \tag{5.61}$$

These solutions consequently enable us to express, for each model, the corresponding function (5.35) as follows

$$L_{R^2}(V_{A,B}) = \frac{4\ 2^{3/4} V_{A,B}^{3/4}}{3^{1/4}}, \tag{5.62}$$

$$L_{R+\beta R^2}(V_{A,B}) = -\frac{2\sqrt{\frac{\beta}{\sqrt{6\beta V_{A,B}+1}-1}}\left(-4\beta V_{A,B} + \sqrt{6\beta V_{A,B}+1} - 1\right)}{\beta}. \tag{5.63}$$

For the tension terms associated with the $f(R)$ models, we obtain first

$$f(R) = R^2 \Rightarrow -\frac{2\,\mathrm{Vol}(X) i}{\hbar}\int_{\bar{s}-\delta s}^{\bar{s}+\delta s} \frac{ds}{C(s)}\left[a^3(3V - 3V_A)\right] \Rightarrow \frac{\mathrm{Vol}(X)}{\hbar}\bar{a}^3 T_0^{f(R)}, \tag{5.64}$$

in this model, the resulting tension term exhibits the identical functional dependence on the potential V as the previously defined term T_0. Consequently, both contributions may be combined into a single effective term. For Starobinsky scenario, we have

$$\begin{aligned} f(R) &= R + \beta R^2 \\ &\Rightarrow -\frac{2\,\mathrm{Vol}(X)i}{\hbar}\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{ds}{C(s)}\left[\frac{a^3\left(3\beta V - 3\beta V_A\right)}{\beta}\right] \\ &\quad + \frac{2\,\mathrm{Vol}(X)i}{\hbar}\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{ds}{C(s)}\left[\frac{a^3\left(\sqrt{6\beta V+1}-\sqrt{6\beta V_A+1}\right)}{\beta}\right] \end{aligned} \tag{5.65}$$

where we can see that the first term has the same functional dependence on V, as mentioned for T_0, so this term must be added to it. However, the second term does not exhibit the same dependence on the potential. To address this discrepancy, it is necessary to define an additional tension term, such that the semiclassical contributions are represented by the expressions

$$R^2 : \Gamma_0 = \mp\frac{\mathrm{Vol}(X)}{\hbar} i\left[L_{R^2}\left(V_B\right) - L_{R^2}\left(V_A\right)\right]\bar{a}^3 + \frac{\mathrm{Vol}(X)}{\hbar}\bar{a}^3 T_0 \tag{5.66}$$

$$\begin{aligned} R + \beta R^2 : \Gamma_0 = &\mp\frac{\mathrm{Vol}(X)}{\hbar} i\left[L_{R+\beta R^2}\left(V_B\right) - L_{R+\beta R^2}\left(V_A\right)\right]\bar{a}^3 + \frac{\mathrm{Vol}(X)}{\hbar}\bar{a}^3 T_0 \\ &+ \frac{\mathrm{Vol}(X)}{\hbar}\frac{\bar{a}^3}{\beta}T_0^{f(R)}. \end{aligned} \tag{5.67}$$

To highlight the contrasting behaviors of the two models, we present in Figure 5.4 the semiclassical contribution for negative potential scenarios. Specifically, we adopt the parameter values $V_B = -5$, $V_A = -1$, $T_0 = 1$, $T_0^{f(R)} = 0.5$ and β[1] $= 10^3$, while choosing positive/negative signs for Γ and the constant field region, respectively, to ensure well defined probability. As we can see, in Starobinsky model, the probability decays faster compared to R^2. For the case of positive potentials, there is no contribution from the L function in any model, so the only difference lies in the additional tension term present in Starobinsky.

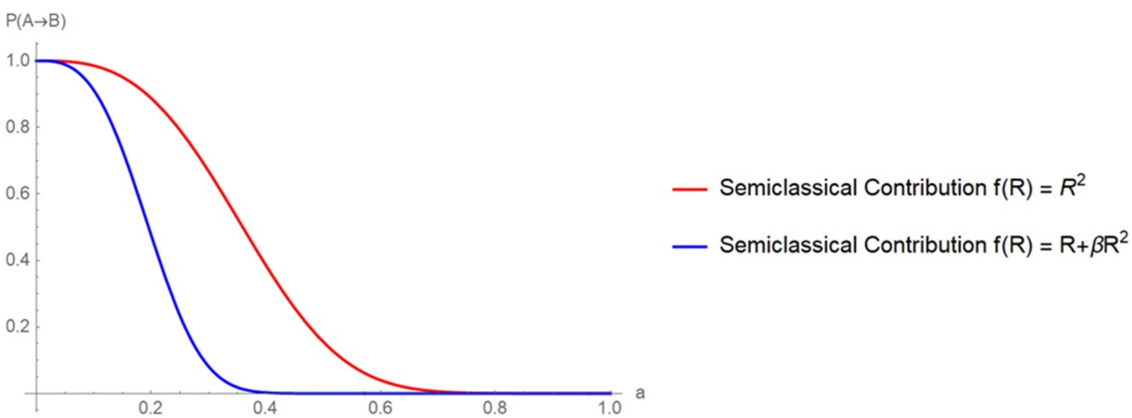

Figure 5.4: Semiclassical contribution for the models $f(R) = R^2$ (Red line) and $f(R) = R + \beta R^2$ (Blue line) with parameters $V_B = -5$, $V_A = -1$, $\beta = 10^3$, $T_0 = 1$, and $T_0^{f(R)} = 0.5$.

Now, considering the first quantum correction as given in (5.38), we identify both a constant tension term and an additional model-dependent tension contribution. For each model under

[1] In the context of the Starobinsky model, the coupling parameter β is approximated by $\beta \sim 1/6M^2$, where M denotes the mass of the inflaton scalar field, which typically lies within the range $M \sim 1.3 \times 10^{-5} M_{Pl}$. Here, M_{Pl} represents the Planck mass. Within the specific set of units established in this thesis, namely $\hbar = c = 8\pi G = 1$, and considering the definition $M_{Pl} = \sqrt{\frac{\hbar c}{8\pi G}}$, the parameter β is projected to be in the range $\sim 10^9$. Consequently, large numerical values for this parameter shall be considered in the subsequent analysis.

consideration, this yields the following expressions

$$\begin{aligned} R^2 &\Rightarrow +\mathrm{Vol}^2(X)\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{ds}{C^2(s)}\left[2\sqrt{\frac{2}{3}}\left(\sqrt{V_A}-\sqrt{V}\right)\right] \\ R+\beta R^2 &\Rightarrow +\mathrm{Vol}^2(X)\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{ds}{C^2(s)}\left[\frac{2\sqrt{\frac{2}{3}}\left(\sqrt{\beta V_A}-\sqrt{\beta V}\right)}{\beta}\right] \end{aligned} \tag{5.68}$$

and as we can see, the term due to R^2 reduces to a constant value. Despite its distinct potential dependence, this contribution may be effectively incorporated into the previously defined T_1 term. In contrast, the Starobinsky counterpart exhibits explicit dependence on the parameter β, consequently, the expressions for the first quantum corrections assume the following forms

$$R^2 : \Gamma_1 = \frac{\mathrm{Vol}(X)}{2}T_1, \tag{5.69}$$

$$R+\beta R^2 : \Gamma_1 = \frac{\mathrm{Vol}(X)}{2}T_1 + \frac{\mathrm{Vol}(X)}{\sqrt{\beta}}T_1^{f(R)}. \tag{5.70}$$

Now, introducing the first correction, in Figure 5.5, considering $V_B = -5$, $V_A = -1$, $T_0 = 1$, $T_0^{f(R)} = 0.5$, $T_1 = 0.1$, $T_1^{f(R)} = 0.5$ preserving the same sign convention, we can se that the incorporation of first quantum correction modifies the probability decay rates, the maximum transition probability $P(A \to B)$ is reduced from one to lower values, with specific reduction depending on the particular $f(R)$ gravity model considered, while preserving the qualitative difference between models observed in the samiclassical contribution, where the Starobinsky model continues to exhibit a more rapid probability decay compared to the R^2 model and leaving the additional Starobinsky tension term as distinguishing feature between the models. Proceeding to the analysis

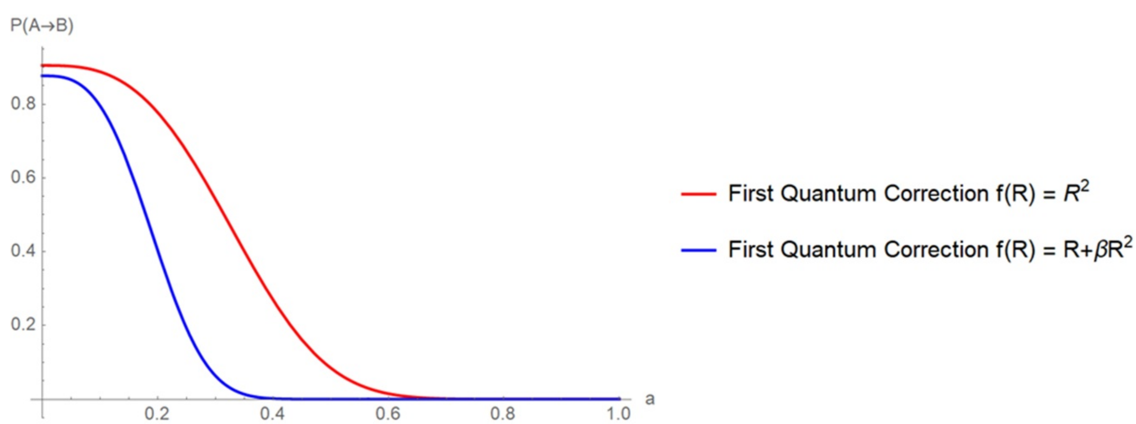

Figure 5.5: First quantum correction for the models $f(R) = R^2$ (Red line) and $f(R) = R + \beta R^2$ (Blue line) with parameters$V_B = -5$, $V_A = -1$, $T_0 = 1$, $T_0^{f(R)} = 0.5$, $T_1 = 0.1$ and $T_1^{f(R)} = 0.5$.

of second order quantum corrections, looking into the tension terms we have

$$\begin{aligned} R^2 : &+\frac{i\hbar}{2}\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{\mathrm{Vol}^3(X)}{C^3(s)}\frac{\sqrt{V}-\sqrt{V_A}}{24\sqrt{6}a^3}ds \\ &+\frac{i\hbar}{2}\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{\mathrm{Vol}^5(X)}{C^5(s)}\frac{4\sqrt{\frac{2}{3}}\left(\sqrt{V}-\sqrt{V_A}\right)}{9a^3}ds, \end{aligned} \tag{5.71}$$

$$
\begin{aligned}
R+\beta R^2 :& + \frac{i\hbar}{2}\int_{\bar{s}-\delta s}^{\bar{s}+\delta s} \frac{\mathrm{Vol}^3(X)}{C^3(s)} \frac{\sqrt{6\beta V+1}-\sqrt{6\beta V_A+1}}{144a^3\beta^6} ds \\
&+ \frac{i\hbar}{2}\int_{\bar{s}-\delta s}^{\bar{s}+\delta s} \frac{\mathrm{Vol}^5(X)}{C^5(s)} \frac{4\left(\sqrt{6\beta V+1}-\sqrt{6\beta V_A+1}\right)}{27a^3\beta^2} ds,
\end{aligned}
\tag{5.72}
$$

where for the case R^2 we observe that both terms have the same dependence on the scale factor and the potential V, following our established methodology for handling tension terms, these contributions may be combined into a single effective term. On the other hand, for the Starobisnky case, we also need to define an additional stress term as was done for the other contributions. In this way, we can define tension terms that take into account the parameter β, let us also note that the dependence on V and the scale factor is the same, so we can define an effective term in the same way with the difference that it will be mediated by a term dependent on β, which leads us to

$$
R^2 : \Gamma_2 = +\frac{\hbar\,\mathrm{Vol}(X)}{\bar{a}^3} T_2, \tag{5.73}
$$

$$
R+\beta R^2 : \Gamma_2 = +\frac{\hbar\,\mathrm{Vol}(X)}{\bar{a}^3} T_2 + +\frac{\hbar\,\mathrm{Vol}(X)}{\bar{a}^3}\left(\frac{3+64\beta^4}{432\beta^6}\right) T_2^{f(R)}. \tag{5.74}
$$

Finally, with the inclusion of the second order quantum correction, in Figure 5.4, considering the parameters $V_B=-5$, $V_A=-1$, $T_0=1$, $T_0^{f(R)}=0.5$, $T_1=0.1$ and $T_1^{f(R)}=0.5$, $T_2=0.001$ and $T_2^{f(R)}=5\times10^{-4}$, we represent this correction for both models. It is readily observable that the avoidance of the singularity is maintained. Furthermore, the characteristic general behavior of the Starobinsky model, which exhibits a lower maximal probability, is preserved.

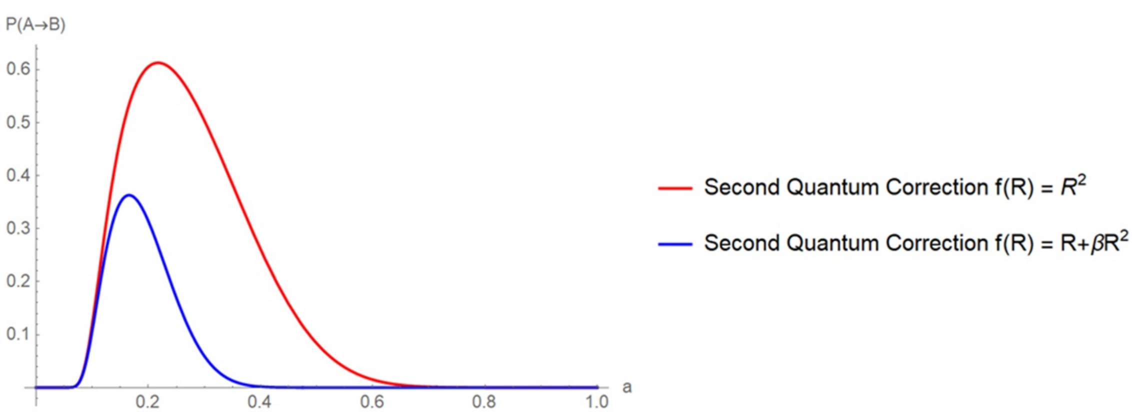

Figure 5.6: Second quantum correction for the models $f(R)=R^2$ (Red line) and $f(R)=R+\beta R^2$ (Blue line) with parameters $V_B=-5$, $V_A=-1$, $T_0=1$, $T_0^{f(R)}=0.5$, $T_1=0.1$ and $T_1^{f(R)}=0.5$, $T_2=0.001$ and $T_2^{f(R)}=5\times10^{-4}$.

5.2.4 Non constant Ricci Scalar

In the preceding section, under the assumption of a constant Ricci scalar, each contribution to the transition probability is reduced to a constant function dependent on the potential V, its derivatives and the parameters of the selected $f(R)$ model, scaled by identical dependence on the scale factor a. Consequently, the general behavior remains analogous. However, if this condition is abandoned, it is not possible to guarantee that the integrals over the constant field regions exhibit the same dependence on the scale factor for all models. The general formalism guides to the expressions

(5.23), (5.25), and (5.28), which may potentially yield more intricate dependencies of the scale factor within constant field regions. This inherent complexity will exert a direct influence on the behavior of the resulting probability. Moreover, in the absence of the condition defined in (5.33), the functional dependence of the curvature scalar R on the scale factor will be dictated by the differential equation (5.22), for which it is only possible to calculate an analytical solution for a limited set of $f(R)$ models. Consequently, the functional dependence of the curvature scalar R on the scale factor will exhibit different behavior across different cases. Furthermore, as a result, the tension terms will also have different dependence on the scale factor, a feature that may or may not alter the overall behavior observed in the case where R is considered constant. Thus, in this section we review the models R^{1+n} that admit an analytical solution to the equation (5.22), and the consequences of considering a non constant Ricci scalar R are analyzed in a general context.

5.2.5 Case R^{1+n}

We now return to the $f(R) = R^{1+n}$ model. So, we have the minisuperspace metric G^{MN} and the remaining fields as

$$G^{MN} = \begin{pmatrix} 0 & -\frac{R^{1-n}}{3a^2n(n+1)} & 0 \\ -\frac{R^{1-n}}{3a^2n(n+1)} & \frac{2R^{2-n}}{3a^3n^2(n+1)} & 0 \\ 0 & 0 & \frac{1}{a^3} \end{pmatrix} \tag{5.75}$$

and

$$\mathcal{V} = a^3\left(\frac{1}{2}nR^{n+1} + V\right). \tag{5.76}$$

Solving the system yields the following expression

$$C^2 = \frac{2\,\mathrm{Vol}^2(X)\left[(2n-1)R^{n+2} + 6RV\right]}{3\left(nR^{n+1} + 2V\right)} \tag{5.77}$$

which allows us to obtain the following relations between variables and the parameter s

$$\frac{da}{ds} = \frac{aR\left(nR^{n+1} + 2V\right)}{2\,\mathrm{Vol}(X)\left[(2n-1)R^{n+2} + 6RV\right]}, \tag{5.78}$$

$$\frac{da}{dR} = \frac{an(n+1)R^n}{(n-2)R^{n+1} + 6V}. \tag{5.79}$$

Leading to the equation

$$\ln(a) = \frac{n\ln\left[(n-2)R^{n+1} + 6V\right]}{n-2} + k', \tag{5.80}$$

this relationship permits the scale factor to be expressed as a function of R, and conversely, R may be written in terms of the scale factor as

$$a = \left[6V + R^{1+n}(-2+n)\right]^{\frac{n}{-2+n}} k \tag{5.81}$$

$$R = \left(\frac{\left(\frac{a}{k}\right)^{\frac{-2+n}{n}} - 6V}{(-2+n)}\right)^{1/1+n}, \tag{5.82}$$

where the integration constant k' is redefined as $k = e^{k'}$. Thus, by considering the general expressions, the semiclassical contribution may be written as

$$\begin{aligned}\Gamma_0 =& \frac{\mp\sqrt{6}\,\mathrm{Vol}(X) i}{\hbar}\left\{\int_{a_0}^{\bar{a}-\delta a} a^2 \frac{\sqrt{(2V_B + R^{1+n}n)\left[(6V_B + R^{1+n}(-1+2n)\right]}}{\sqrt{R}} da \right.\\ &\left. - \int_{a_0}^{\bar{a}-\delta a} a^2 \frac{\sqrt{(2V_A + R^{1+n}n)\left[(6V_A + R^{1+n}(-1+2n)\right]}}{\sqrt{R}} da \right\} \\ &+ \frac{\mathrm{Vol}(X)}{\hbar}\bar{a}^3 T_0 + \frac{2\,\mathrm{Vol}(X) i}{\hbar}\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{ds}{C(s)}\left(-\frac{1}{2}a^3 R^{1+n} n + \frac{1}{2}a^3 R^{1+n} n\mid_{\phi_A}\right)\end{aligned} \tag{5.83}$$

When R is expressed in terms of the scale factor, the integrals over the constant field regions do not admit analytical solutions. However, they remain manageable for numerical evaluation. To proceed, the tension term, which exhibits an explicit dependence on the parameter n, is first examined. Under the condition that $k = k_A$ this expression is written as

$$T_0^{f(R)} \sim +\frac{2\,\mathrm{Vol}(X) i}{\hbar}\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{ds}{C(s)}\left(\frac{3n}{n-2}\right) a^3\left(V - V_A\right). \tag{5.84}$$

Now, to expose the behavior of the semiclassical contributions as a function of the parameter n, and to analyze the effects of sign variations on the tension terms, we present in Figure 5.7 a comprehensive set of plots, that encompass both negative and positive potential scenarios and the set of parameters $k_A = k_B = 1$, $\mathrm{Vol}(X) = 1$ $V_B = -5, 5$, $V_A = -1, 10$, $T_0 = 1$ and $T_0^{f(R)} = 0.05$. In the case of positive potentials, the integrals over the constant potential regions do not contribute to the transition probability within the parameter range $0 < n < 2$. Consequently, the probability amplitude is dominated by the tension terms in this interval. However, for values of $n > 2$, these integrals become non zero and are well defined, thereby contributing to the probability. By contrast, for negative potentials, there is always a non vanishing contribution from these integrals to the transition probability, irrespective of the value of n.

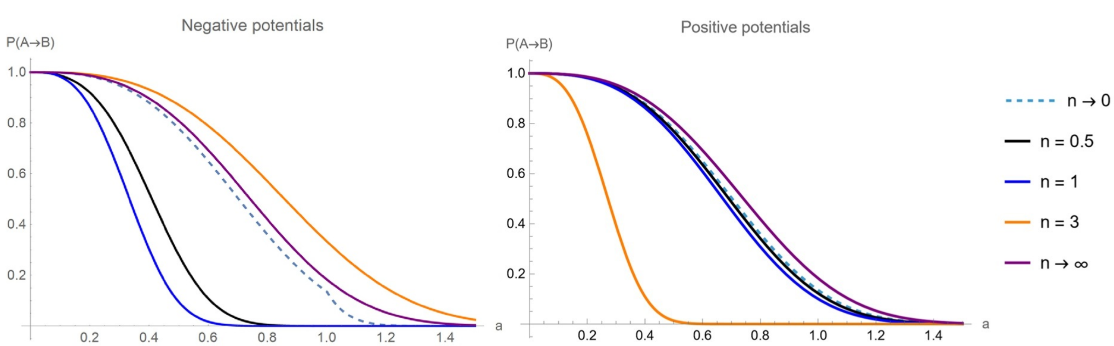

Figure 5.7: Semiclassical contributions for the power-law $f(R) = R^{1+n}$ model, varying values of the exponent n. The different curves correspond to: $n \to 0$ (dashed line), $n = 0.5$ (black line), $n = 1$ (blue line), $n = 3$ (orange line), and $n \to \infty$ (purple line). Both panels share the fixed parameters: $k_A = k_B = 1$, $\mathrm{Vol}(X) = 1$, with potential values $V_B = \{-5, 5\}$, $V_A = \{-1, 10\}$, and tension parameters $T_0 = 1$ and $T_0^{f(R)} = 0.05$. The left/right panels illustrate the negative/positive potential scenarios respectively.

We can se that for negative potentials the transition probabilities exhibit faster decay as n approaches 2 from below ($n < 2$). The critical value at $n = 2$ marks a singular point in our analysis where the tension term associated with the $f(R)$ modification undergoes a sign change.

Beyond this point ($n > 2$), the probability decay rate eventually surpass those observed in the $n \to 0$ limit. As n increases further, the probabilities approach an asymptotic upper bound in the $n \to \infty$ limit. On the other hand for positive potentials, while the qualitative behavior mirrors that observed for negative potentials, the effects are attenuated. Specifically, within the range $0 < n < 2$, the transition probabilities remain close to the $n \to 0$ limit, as a consequence of the dominant contribution of only the tension terms. Upon entering the $n > 2$ region, the previously vanish contributions from the integrals over constant field regions enter, resulting in probabilities that initially decay more rapidly but, as n continues to increase, these probabilities approach an asymptotic upper bound. Continuing with the first quantum correction, taking the expression (5.25), we have

$$\begin{aligned}\Gamma_1 = &\mathrm{Vol}(X)\left\{\int_{a_0}^{\bar{a}-\delta a}\left(\frac{-2R+3V_B^{(2)}}{aR}\right)da - \int_{a_0}^{\bar{a}-\delta a}\left(\frac{-2R+3V_A^{(2)}}{aR}\right)da\right\}\\ &+\frac{\mathrm{Vol}(X)}{2}T_1\\ &+\mathrm{Vol}(X)\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{ds}{C^2(s)}\left(-\frac{2}{3}R+\frac{2}{3}R\Big|_{\phi_A}\right)\end{aligned} \tag{5.85}$$

Given the form of R, the tension term corresponding to $f(R)$ in the first correction will have a different form for each value of n, unlike the semiclassical contribution which keeps the dependence on the scale factor due to the appropriate consideration of the integration constant for the relationship between the scale factor and the curvature scalar. Since this term cannot be expressed in the separable form $N(\phi)O(a)$ and exhibits a distinct structure for each value of n, a general approximation scheme for a generalized tension term is not possible. Consequently, we will focus on the specific case $n = 1$ to investigate the impact of the quantum corrections without considering that R is constant.

5.2.6 Pure quadratic gravity

To properly account for quantum corrections in the modified gravity model $f(R) = R^{1+n}$, different analytical treatments are required for each value of n as shown above. In this section, we specialize to the case $n = 1$ to examine its specific effects on transition probabilities, particularly focusing on the integral contributions from constant field regions. In this manner, We have the scalar curvature and the scale factor related[2] by

$$R = \sqrt{6V + \frac{k}{a}}. \tag{5.86}$$

Such that the semiclassical contribution (5.83) for the transition probability can be expressed as

$$\begin{aligned}\Gamma_0 = \mp\, &\frac{\sqrt{6}\,\mathrm{Vol}(X)i}{\hbar}\left[\int_{\bar{a}_0}^{\bar{a}-\delta a} a^{5/4}\frac{\sqrt{(12aV_B+k)\,(8aV_B+k)}}{(6aV_B+k)^{1/4}}da\right.\\ &\left.-\int_{\bar{a}_0}^{\bar{a}-\delta a} a^{5/4}\frac{\sqrt{(12aV_A+k)\,(8aV_A+k)}}{(6aV_A+k)^{1/4}}da\right]\\ &+\frac{\mathrm{Vol}(X)\bar{a}^3T_0}{\hbar},\end{aligned} \tag{5.87}$$

where, in the third line, a tension term including both contributions is defined given that them has the same dependence on V. Continuing the analysis with higher order terms, the first quantum

[2] In this expression, the term $-k$ is substituted by $+k$ for the purpose of simplification, facilitating the consideration of the condition $k > 0$.

correction, Γ_1, defined in (5.85), can be initially written as

$$\begin{aligned}\Gamma_1 = \mathrm{Vol}(X)\Bigg(&\int_{a_0}^{\bar{a}-\delta a} -\frac{2}{a} + \frac{3V_B^{(2)}}{a\sqrt{\frac{k}{a}+6V_B}}da \\ &-\int_{a_0}^{\bar{a}-\delta a} -\frac{2}{a} + \frac{3V_A^{(2)}}{a\sqrt{\frac{k}{a}+6V_A}}da\Bigg) + \mathrm{Vol}(X)T_1 \\ &-\mathrm{Vol}(X)\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{ds}{C^2(s)}\left(\frac{2}{3}\sqrt{6V+\frac{k}{a}} - \frac{2}{3}\sqrt{6V_A+\frac{k}{a}}\right).\end{aligned} \tag{5.88}$$

Upon integration, the expression becomes

$$\begin{aligned}\Gamma_1 = \mathrm{Vol}(X)\Bigg[&-2\ln(a) + \sqrt{6}\frac{V_B^{(2)}}{\sqrt{V_B}}\,\mathrm{ArcTanh}\left(\sqrt{\frac{k}{6V_B a}+1}\right)\Bigg|_{\bar{a}_0}^{\bar{a}-\delta a} \\ &+2\ln(a) - \sqrt{6}\frac{V_A^{(2)}}{\sqrt{V_A}}\,\mathrm{ArcTanh}\left(\sqrt{\frac{k}{6V_A a}+1}\right)\Bigg|_{\bar{a}_0}^{\bar{a}-\delta a}\Bigg] \\ &+\mathrm{Vol}(X)T_1 \\ &-\mathrm{Vol}(X)\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{ds}{C^2(s)}\frac{2}{3}\left(\sqrt{6V+\frac{k}{a}} - \sqrt{6V+\frac{k}{a}}\Bigg|_{\phi_A}\right).\end{aligned} \tag{5.89}$$

It is observed that a term involving $\ln(a)$ appears, a feature also present in the first quantum correction calculated for General Relativity and for the approach employed in Section 5.2.1. However, in the present context, this term naturally cancels without requiring the imposition of any auxiliary constraints, which differs from those prior cases. Considering the integral term in the non constant potential region, certain assumptions are required to approximate the root term and define an additional tension term. For this purpose, the root term is rewritten as:

$$\begin{aligned}\sqrt{\frac{k}{a}+6V} &= \sqrt{6V}\sqrt{\frac{k}{6Va}+1} \\ &\approx \sqrt{6V}\left(\sqrt{\frac{k}{6Va}} + \frac{\sqrt{6Va}}{2\sqrt{k}}\right) = \sqrt{\frac{k}{a}} + \frac{3V}{\sqrt{k}}\sqrt{a},\end{aligned} \tag{5.90}$$

where the condition $\frac{k}{6Va} \gg 1$ is considered. It is noted that the first term of this expansion possesses a functional form akin to the integral previously neglected in the semiclassical contribution. Consequently, for analogous reasons, this term is also neglected, retaining the second term of the expansion, which allows the definition of an additional tension term. Furthermore, the term subjected to expansion within the tension term is observed to be identical to the argument of the ArcTanh function. Thus, under the asymptotic condition where $\frac{k}{6V_{A,B}a} \gg 1$ and $a \ll 1$, the ArcTanh function can be approximated as

$$\mathrm{ArcTanh}\left(\sqrt{\frac{k}{6Va}+1}\right) \approx -\frac{\pi i}{2} + \sqrt{\frac{6Va}{k}}. \tag{5.91}$$

This approximation allows for the selection of limit $a_0 = 0$. Therefore, the first quantum correction Γ_1 is finally approximated by

$$\Gamma_1 = 6\,\mathrm{Vol}(X)\left[\left(V_B^{(2)} - V_A^{(2)}\right)\sqrt{\frac{\bar{a}}{k}}\right] + \mathrm{Vol}(X)T_1 + \mathrm{Vol}(X)\sqrt{\bar{a}}T_1^{f(R)}. \tag{5.92}$$

For the subsequent order, $O(\hbar^2)$, the second quantum correction, the following expressions are established

$$\nabla^2\left(\nabla^2\mathcal{V}\right)=\frac{V^{(4)}}{a^3}, \tag{5.93}$$

and

$$\left[\nabla\left(\nabla^2\mathcal{V}\right)\right]^2=\frac{V^{(3)2}}{a^3}+\frac{4R}{27a^3}. \tag{5.94}$$

Furthermore, the auxiliary functions $F(a,V_{A,B})$ and $G(a,V_{A,B})$ are defined as

$$F(a,V_{A,B})=\sqrt{\frac{27}{2}}\int\frac{\sqrt{a}\sqrt{\frac{\sqrt{a}(k+8aV_{A,B})}{(k+12aV_{A,B})\sqrt{k+6aV_{A,B}}}}}{a^4\sqrt{k+6aV_{A,B}}}da, \tag{5.95}$$

and

$$\begin{aligned}G(a,V_{A,B})=&\int\frac{\sqrt{\frac{k}{6a}+V_{A,B}}\left(4\sqrt{\frac{k}{a}+6V_{A,B}}+27V^{(3)}_{A,B}\right)}{2a^3(6aV_{A,B}+k)}\times\\&\times\left[\frac{8aV_{A,B}+k}{\sqrt{\frac{k}{a}+6V_{A,B}}(12aV_{A,B}+k)}\right]^{3/2}da,\end{aligned} \tag{5.96}$$

such that the second quantum correction Γ_2 can be expressed as

$$\begin{aligned}\Gamma_2=\pm\frac{i\hbar\,\mathrm{Vol}(X)}{2}&\left[V_B^{(4)}F\left(a,V_B\right)\Big|_{\bar{a}_0}^{\bar{a}-\delta a}-V_A^{(4)}F\left(a,V_A\right)\Big|_{\bar{a}_0}^{\bar{a}-\delta a}\right.\\&\left.+G\left(a,V_B\right)|_{\bar{a}_0}^{\bar{a}-\delta a}-G\left(a,V_A\right)|_{\bar{a}_0}^{\bar{a}-\delta a}\right]\\&+\frac{\hbar\,\mathrm{Vol}(X)T_2}{\bar{a}^3}\\&+\frac{i\hbar}{2}\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\mathrm{Vol}^5(X)\frac{ds}{C^5(s)}\left(\frac{4}{27}\right)\left(\frac{1}{a^3}\right)\left(R-R\,|_{\phi_A}\right).\end{aligned} \tag{5.97}$$

Following the established approximation procedure utilized for the previous contributions, the integral in the last line is approximated, yielding the refined expression

$$\begin{aligned}\Gamma_2=\pm\frac{i\hbar\,\mathrm{Vol}(X)}{2}&\left[V_B^{(4)}F\left(a,V_B\right)\Big|_{\bar{a}_0}^{\bar{a}-\delta a}-V_A^{(4)}F\left(a,V_A\right)\Big|_{\bar{a}_0}^{\bar{a}-\delta a}\right.\\&\left.+G\left(a,V_B\right)|_{\bar{a}_0}^{\bar{a}-\delta a}-G\left(a,V_A\right)|_{\bar{a}_0}^{\bar{a}-\delta a}\right]\\&+\frac{\hbar\,\mathrm{Vol}(X)T_2}{\bar{a}^3}\\&+\hbar\,\mathrm{Vol}(X)\frac{1}{\sqrt{\bar{a}^5}}T_2^{f(R)},\end{aligned} \tag{5.98}$$

where a supplementary tension term, $T_2^{f(R)}$, has been explicitly defined. To illustrate the behavior of the transition probability and its associated quantum corrections, Figure 5.8 presents a plot generated using the following parameter values $k=1$, $V_B=5$, $V_A=10$, $V_B^{(2)}=0.15$, $V_A^{(2)}=0.5$, $V_B^{(3)}=0.6$, $V_A^{(3)}=0.2$, $V_B^{(4)}=0.25$, $V_A^{(4)}=0.2$, $T_0=1$, $T_0^{f(R)}=0.1$, $T_1=0.1$, $T_1^{f(R)}=0.001$, $T_2=0.0005$, and $T_2^{f(R)}=0.00001$. From the graph presented in the figure, it is evident that, within a suitable range of the scale factor a that validates the applied approximations, the semiclassical contribution exhibits a maximal probability at zero and subsequently undergoes decay. The inclusion of the first quantum correction serves to reduce this maximal probability value and modifies the form of the transition probability. Furthermore, the second quantum correction dictates that the maximal probability value is situated at a non zero, finite value of the scale factor.

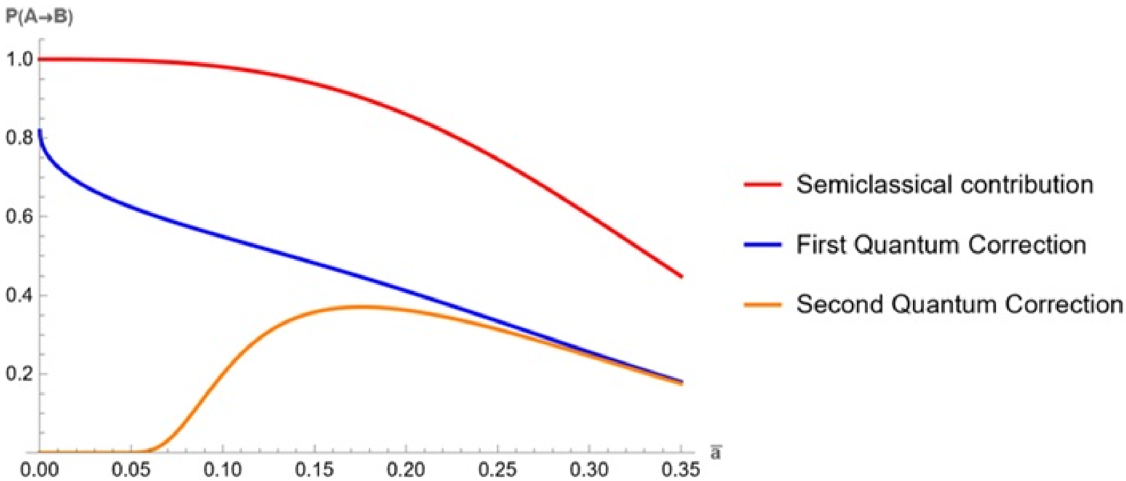

Figure 5.8: $k = 1$, $V_B = 5$, $V_A = 10$, $V_B^{(2)} = 0.15$, $V_A^{(2)} = 0.5$, $V_B^{(3)} = 0.6$, $V_A^{(3)} = 0.2$, $V_B^{(4)} = 0.25$, $V_A^{(4)} = 0.2$, $T_0 = 1$, $T_0^{f(R)} = 0.1$, $T_1 = 0.1$, $T_1^{f(R)} = 0.001$, $T_2 = 0.0005$, and $T_2^{f(R)} = 0.00001$.

5.3 Limitations

As demonstrated in the preceding sections, the flat FLRW case in the constant R condition regime allows, in principle, the analysis of any $f(R)$ model that satisfies the espression (5.33) and permits the derivation of an expression for the Hubble parameter. If the same principle is applied to the closed FLRW metric, it becomes necessary to compare the following expressions

$$\frac{da}{ds} = \frac{\left(a^2R - 6\right)\left[a^2(f - 2V) + \left(6 - a^2R\right) f_R\right]}{2a\,\mathrm{Vol}(X)\left[\left(a^2R - 6\right)(3f - 2Rf_R - 6V) + 6a^2V^{(1)2}\right]} \tag{5.99}$$

and

$$\frac{dR}{ds} = \frac{-3a^4(f - 2V)^2 + 4a^2\left(a^2R - 3\right) f_R(f - 2V) + \left(36 - a^4R^2\right) f_R{}^2}{2a^2\,\mathrm{Vol}(X) f_{RR}\left[\left(a^2R - 6\right)(3f - 2Rf_R - 6V) + 6a^2V^{(1)2}\right]}, \tag{5.100}$$

where the new condition for satisfying $dR = 0$ while maintaining $da \neq 0$ is given by

$$(6V + Rf_R - 3f) + \frac{6}{a^2} = 0. \tag{5.101}$$

It can be observed from the previous expression that the condition established for the flat case is modified by a term dependent on the scale factor, thus precluding the curvature scalar R from being constant.

On the other hand, if we want to consider the treatment developed in the section 5.2.4, it becomes necessary to address the differential equation

$$\frac{da}{dR} = \frac{a\left(a^2R - 6\right) f_{RR}}{\left(a^2R + 6\right) f_R - 3a^2(f - 2V)}. \tag{5.102}$$

Although this expression allows for the general formulation of the semiclassical contributions and the quantum corrections as

$$\begin{aligned}\Gamma_0 =& \pm 2\sqrt{\frac{3}{2}}\frac{\mathrm{Vol}(X)i}{\hbar}\left\{\int_{a_0}^{\bar{a}-\delta a} a^2\left(-3f+6V_B+2Rf_R\right)\times\right.\\ &\times\sqrt{\frac{-a^2f+2a^2V_B+\left(-6+a^2R\right)f_R}{\left(-6+a^2R\right)\left(-3f+6V_B+2Rf_R\right)}}da\\ &\left.-\int_{a_0}^{\bar{a}-\delta a} a^2\left(-3f+6V_A+2Rf_R\right)\sqrt{\frac{-a^2f+2a^2V_A+\left(-6+a^2R\right)f_R}{\left(-6+a^2R\right)\left(-3f+6V_A+2Rf_R\right)}}da\right\}\\ &+\frac{\mathrm{Vol}(X)}{\hbar}\bar{a}^3T_0\\ &+\frac{2\,\mathrm{Vol}(X)i}{\hbar}\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{ds}{C(s)}\left[\frac{a^3}{2}\left(f-Rf_R\right)+3f_Ra\right.\\ &\left.-\frac{a^3}{2}\left(f-Rf_R\right)\Big|_{\phi=\phi_A}-3f_Ra\left.\right|_{\phi=\phi_A}\right],\end{aligned} \tag{5.103}$$

$$\begin{aligned}\Gamma_1 =& \mathrm{Vol}(X)\left\{\int_{a_0}^{\bar{a}-\delta a}\frac{3f_{RR}^2\left[\left(2-a^2R\right)+a^2V_B^{(2)}\right]+f_R\left[a^2f_{RR}+\left(-6+a^2R\right)f_{RRR}\right]}{a\left(-6+a^2R\right)f_{RR}^2}da\right.\\ &\left.-\int_{a_0}^{\bar{a}-\delta a}\frac{3f_{RR}^2\left[\left(2-a^2R\right)+a^2V_A^{(2)}\right]+f_R\left[a^2f_{RR}+\left(-6+a^2R\right)f_{RRR}\right]}{a\left(-6+a^2R\right)f_{RR}^2}da\right\}\\ &+\frac{\mathrm{Vol}(X)}{2}T_1\\ &+\mathrm{Vol}^2(X)\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{ds}{C^2(s)}\left[\frac{f_R\left(f_{RR}+Rf_{RRR}\right)}{3f_{RR}^2}-R-\frac{2f_Rf_{RRR}}{a^2f_{RR}^2}\right.\\ &\left.-\frac{f_R\left(f_{RR}+Rf_{RRR}\right)}{3f_{RR}^2}\Big|_{\phi=\phi_A}+R|_{\phi=\phi_A}-\frac{2f_Rf_{RRR}}{a^2f_{RR}^2}\Big|_{\phi=\phi_A}\right]\end{aligned} \tag{5.104}$$

and defining the auxiliary terms are as

$$\begin{aligned}U =& -24f_{RR}^4f_{RRR}+2f_Rf_{RR}^2\left\{-3\left(-14+a^2R\right)f_{RRR}^2\right.\\ &\left.+f_{RR}\left[a^2f_{RRR}+2\left(-12+a^2R\right)f_{RRRR}\right]\right\}\\ &+2f_R^2\left\{6\left(-6+a^2R\right)f_{RRR}^3-2f_{RR}f_{RRR}\left[a^2f_{RRR}+3\left(-6+a^2R\right)f_{RRRR}\right]\right.\\ &\left.+f_{RR}^2\left[a^2f_{RRRR}+\left(-6+a^2R\right)f_{RRRRR}\right]\right\},\end{aligned} \tag{5.105}$$

and

$$\begin{aligned}W =& +3f_{RR}^6\left[-16a^2f_{RR}+8\left(-6+a^2R\right)f_{RRR}\right]\\ &-4\left(-6+a^2R\right)f_R^2f_{RR}^2\left[2a^2f_{RR}+\left(12-a^2R\right)f_{RRR}\right]\left(-2f_{RRR}^2+f_{RR}f_{RRRR}\right)\\ &+2\left(-6+a^2R\right)^2f_R^3\left(-2f_{RRR}^2+f_{RR}f_{RRRR}\right)^2+2f_Rf_{RR}^4\left\{4a^4f_{RR}^2\right.\\ &+\left(252-48a^2R+a^4R^2\right)f_{RRR}^2\\ &\left.-4f_{RR}\left[a^2\left(-12+a^2R\right)f_{RRR}-3\left(-6+a^2R\right)f_{RRRR}\right]\right\},\end{aligned} \tag{5.106}$$

we will have

$$\begin{aligned}
\Gamma_2 = \pm\, \frac{i\hbar\,\mathrm{Vol}(X)}{2} \Bigg\{ & \int_{a_0}^{\bar{a}-\delta_a} \frac{\left(U + 9a^2 f_{RR}^6 V_B^{(4)}\right)}{\sqrt{6}a^4 \left(-6+a^2R\right) f_{RR}^6} \sqrt{\frac{-a^2 f + 2a^2 V_B + \left(-6+a^2R\right) f_R}{\left(-6+a^2R\right)\left(-3f+6V_B+2Rf_R\right)}} da \\
& + \int_{a_0}^{\bar{a}-\delta a} \frac{\left(W + 27a^4 f_{RR}^2 V_B^{(3)2}\right)}{2\sqrt{6}a^6 \left(-6+a^2R\right) f_{RR}^8} \left[\frac{-a^2 f + 2a^2 V_B + \left(-6+a^2R\right) f_R}{\left(-6+a^2R\right)\left(-3f+6V_B+2Rf_R\right)}\right]^{\frac{3}{2}} da \\
& - \int_{a_0}^{\bar{a}-\delta a} \frac{\left(U + 9a^2 f_{RR}^6 V_A^{(4)}\right)}{\sqrt{6}a^4 \left(-6+a^2R\right) f_{RR}^6} \sqrt{\frac{-a^2 f + 2a^2 V_A + \left(-6+a^2R\right) f_R}{\left(-6+a^2R\right)\left(-3f+6V_A+2Rf_R\right)}} da \Bigg\} \\
& - \int_{a_0}^{\bar{a}-\delta a} \frac{\left(W + 27a^4 f_{RR}^2 V_A^{(3)2}\right)}{2\sqrt{6}a^6 \left(-6+a^2R\right) f_{RR}^8} \left[\frac{-a^2 f + 2a^2 V_A + \left(-6+a^2R\right) f_R}{\left(-6+a^2R\right)\left(-3f+6V_A+2Rf_R\right)}\right]^{\frac{3}{2}} da \Bigg\} \\
& + \frac{i\hbar}{2} \int_{s_0}^{s-\delta s} \frac{\mathrm{Vol}^3(X) ds}{C^3(s)} \left(\frac{1}{a^3}\right) \left(V^{(4)} - V_A^{(4)}\right) \\
& + \frac{i\hbar}{2} \int_{s_0}^{\bar{s}-\delta_s} \frac{\mathrm{Vol}^5(X) ds}{C^5(s)} \left(\frac{1}{a^3}\right) \left(V^{(3)2} - V_A^{(3)2}\right) \\
& + \frac{i\hbar}{2} \int_{\bar{s}-\delta s}^{\bar{s}+\delta s} \frac{\mathrm{Vol}^3(X) ds}{C^3(s)} \left(\frac{1}{9a^5}\right) \left(\frac{U}{f_{RR}^6} - \frac{U}{f_{RR}^6}\,|_{\phi=\phi_A}\right) \\
& + \frac{i\hbar}{2} \int_{\bar{s}-\delta s}^{\bar{s}+\delta s} \frac{\mathrm{Vol}^5(X) ds}{C^5(s)} \left(\frac{1}{27a^7}\right) \left(\frac{W}{f_{RR}^8} - \frac{W}{f_{RR}^8}\,|_{\phi=\phi_A}\right),
\end{aligned} \tag{5.107}$$

the differential equation itself does not admit an analytical solution, even for relatively simple models such as $f(R) = R^2$. Consequently, the integration over the constant field regions is not possible, and the tension terms cannot be explicitly defined.

Chapter 6

Final Remarks

In this thesis we establish a rigorous general formalism for calculating vacuum transition probabilities within a purely Lorentzian framework. By bypassing the need for Euclidean Wick rotations, this approach offers a direct method to address quantum tunneling phenomena in cosmological contexts, utilizing the canonical quantization of the Hamiltonian constraint to derive the Wheeler-DeWitt equation.

The core of this methodology lies in the application of the Wentzel-Kramers-Brillouin (WKB) approximation to the wave functional of the universe. This semiclassical expansion allows for the systematic separation of the action into a classical component and subsequent higher-order quantum corrections. A critical aspect of this derivation is the use of integral curves along classical trajectories in the configuration space, which facilitates the resolution of the Hamilton-Jacobi-type equations that arise at each order of the expansion parameter. This procedure effectively reduces the problem of finding the wave functional to evaluating integrals along these specific paths, thereby rendering the calculation of transition amplitudes tractable.

A significant conceptual contribution is the interpretation of the transition probability. Rather than relying on a probabilistic measure defined over the entire superspace, which remains elusive in quantum cosmology, the formalism adopts a conditional probability approach. The transition probability is defined as the squared modulus of the ratio between the wave functional evaluated at a true vacuum configuration and the wave functional evaluated at a false vacuum configuration. This definition provides a physically meaningful quantity that describes the relative likelihood of tunneling between metastable states.

The explicit derivation of the decay rate reveals a hierarchical structure composed of the semiclassical contribution followed by the first and second quantum corrections. First, the Semiclassical Contribution, is the leading-order term preserves the functional form associated with classical action integrals. In the thin-wall approximation, this contribution separates into bulk terms, which depend on the potential difference between the minima, and a tension term that encapsulates the the scalar field as it transitions across the potential barrier. Importantly, the formalism demonstrates that at this order, the tension term corresponds to the bubble tension identified in Euclidean approaches, confirming the consistency of the Lorentzian method with established semiclassical results. The subsequent consideration of quantum corrections introduce additional complexity. The first-order correction manifests primarily as a modification to the tension, involving second derivatives of the potential. The second-order correction further expands this structure, introducing terms dependent on higher-order derivatives of the potential and the gradients of the first-order correction itself.

A crucial feature identified in this general analysis is the role of the spatial volume. The formalism indicates that the volume of the spatial slice appears as a global factor in the decay rate expressions, suggesting that the results can be generalized to non-compact topologies by considering finite spatial regions. Furthermore, the analysis of the tension terms reveals that, generally, the number of independent tension parameters increases with the order of the correction, although symmetries in specific metric choices may reduce this complexity.

It is also worth noting a potential limitation regarding modified gravity theories. The definition of tension terms relies on the ability to separate the integrals across the domain wall into functions of the scalar field and functions of the metric. The formalism anticipates that certain complex modified gravity models, such as specific $f(R)$ theories, might not satisfy this separability condition easily, a challenge that is addressed in the subsequent applications of this framework.

So, firstly we focus on gravity in $(2+1)$ dimensión, this analysis functions as laboratory. While General Relativity in three spacetime dimensions lacks local propagating degrees of freedom rendering it a "toy model" compared to the realistic four-dimensional theory, its mathematical tractability allows for an exact quantization in many contexts. In thi way, we rigorously test the WKB expansion method and, most importantly, investigate how different factorization choices in the Hamiltonian formulation influence quantum predictions.

The analysis commences with the Flat FLRW Metric, where the study introduces a pivotal comparison between two distinct factorization schemes for the Hamiltonian constraint. Considering a factorization $1/a^2$, the Hamiltonian is treated without considering the inverse scale factor in the momentum terms. The results indicate that while the semiclassical contribution exhibits regular behavior, the inclusion of quantum corrections leads to a transition probability that approaches unity as the universe's size vanishes. This suggests that, under this specific algebraic arrangement, the most probable initial configuration remains the spatial singularity. The second approach does not factors the inverse scale factor within the lapse function. This algebraic difference, while classically equivalent, alters the operator ordering upon quantization. Crucially, the analysis reveals that including the second-order quantum correction in this scheme suppresses the transition probability to zero at the origin. This finding is of paramount physical significance, as it demonstrates that specific quantum corrections can provide a mechanism to avoid the initial singularity, predicting instead that the universe emerges with a finite, non-zero size.

We extend the method to the Closed FLRW Metric, representing a universe with positive spatial curvature. Here, the results highlight the topological distinctions inherent to the dimensionality. Unlike the flat case, the imposition of boundary conditions at the origin requires specific consistency constraints on the potential and its derivatives to eliminate logarithmic divergences in the quantum corrections. When these conditions are met, the probability distribution is shown to initiate from a value strictly less than unity, reinforcing the role of quantum effects in modifying the likelihood of singular initial states.

When consider anisotropic cosmologies, specifically the Bianchi Type I and Type III metrics. For Bianchi Type I, the analysis demonstrates that for this metric, the scale factors associated with different spatial directions remain proportional. Consequently, the results are mathematically identical to those obtained for the flat FLRW metric, confirming that simple anisotropy does not intrinsically alter the tunneling behavior in this dimension without additional geometric complexity. Considering Bianchi Type III, this metric provides a more robust test of anisotropy. A key discovery here is the non-trivial behavior of the isotropy limit. While the semiclassical contribution for the Bianchi Type III metric smoothly recovers the flat FLRW result as the anisotropy parameter vanishes, this correspondence breaks down at the level of quantum corrections. The study shows that the quantum corrections retain a persistent dependence on the anisotropy parameter, preventing a full recovery of the isotropic result. This implies that quantum corrections are sensitive to the global topological structure of the minisuperspace, differentiating between isotropic and anisotropic origins even in limits where they classically converge.

In summary, for gravity in $(2+1)$ dimensions, we establish two fundamental conclusions that guide the subsequent analysis in higher dimension. First, it proves that the specific algebraic factorization of the Hamiltonian constraint is not merely a formal choice but a determinant factor in the behavior of quantum corrections, particularly regarding the resolution of the initial singularity. Second, it reveals that quantum corrections can break the degeneracy between models that are connected via classical limits, as evidenced by the discrepancy between the anisotropic and isotropic results.

Then considering gravity in $(3+1)$, this scenario represents the culmination of the application of the Lorentzian formalism to General Relativity, extending the insights gained from lower-dimensional models to the physically realistic four-dimensional spacetime. We examnie vacuum transition probabilities across different cosmological geometries, revealing a fundamental distinction between isotropic and anisotropic scenarios regarding the resolution of the initial singularity.

As well for the $(2+1)$ dimensional case, the analysis of isotropic Universes, we consider the closed and flat FLRW metrics, yielding to the most profound physical implication of this thesis. The study establishes that at the semiclassical level, the transition probability distribution attains its maximum value precisely at the point corresponding to a zero scale factor.This implies that, classically, the most probable origin of the universe is the initial spatial singularity. The introduction of quantum corrections fundamentally alters this narrative. While the first-order correction merely modulates the amplitude without shifting the maximum, the second-order correction introduces a term that diverges as the scale factor approaches zero. When combined with the semiclassical term, this creates a competitive mechanism: the semiclassical contribution dominates at large scales, while the second quantum correction dominates at small scales, suppressing the probability to zero at the origin. Consequently, the probability distribution peaks at a finite, non-zero value of the scale factor. This result provides a robust prediction that, within this quantum framework, the universe is most likely to emerge with a finite initial size, effectively avoiding the classical singularity. It is interesting that the change of behaviour appears at second order in the quantum correction terms, the same occurs when computing quantum corrections to the Schrödinger equation coming from the Klein-Gordon equation as shown in [182]. Thus, since the WDW equation is a Klein-Gordon type equation in superspace we obtain a consistent result in this regard.

When consider anisotropic universes, via the Bianchi Type III and Kantowski-Sachs metrics, we found a critical counterpoint to the isotropic results. A key finding in this section is the reinterpretation of the singularity. In the Bianchi Type III analysis, the point of maximum semiclassical probability (where the primary scale factor vanishes) does not correspond to a true spatial singularity where all dimensions collapse. Instead, due to the specific relationships between the metric variables derived from the field equations, this point represents a "bounce" scenario or a configuration where one spatial dimension vanishes while others diverge. Therefore, while the second quantum correction successfully suppresses the probability at this specific point, it does not strictly constitute the avoidance of a spacetime singularity in the same sense as the isotropic case. This conclusion is reinforced by the analysis of the Kantowski-Sachs metric. Here, the probability suppression occurs at a configuration where the radial component vanishes, but the angular components remain non-zero. This confirms that the mechanism of "avoidance" observed in anisotropic models is geometrically distinct from the resolution of the singularity found in FLRW cosmologies.

Furthermore, we want to highlight a subtle but significant feature regarding the isotropy limit. The analysis demonstrates that while the semiclassical results for the anisotropic Bianchi III metric smoothly converge to the flat FLRW results as the anisotropy parameter vanishes, this correspondence breaks down at the level of quantum corrections, as was also seen in the three-dimensional case. The structure of the minisuperspace for the anisotropic metric differs sufficiently from the isotropic one such that the Laplacian operators do not coincide in the limit. Consequently, the quantum corrections retain a memory of the anisotropic structure, leading to results that differ by specific constants from the purely isotropic derivation. This underscores that quantum corrections are highly sensitive to the global topological definition of the configuration space.

So,in this way we stablish that the avoidance of the initial spatial singularity via second-order quantum corrections is a phenomenon strictly unique to the isotropic universe. In anisotropic scenarios, while quantum effects still modify the probability distributions and suppress specific configurations, the geometric complexity precludes a simple interpretation of singularity resolution.

Afterward, we expan the scope of the research beyond standard General Relativity, applying the established Lorentzian formalism to the class of modified gravity theories known as $f(R)$ gravity. This extension is non-trivial, as higher-order curvature terms typically introduce fourth-order differential equations that complicate the Hamiltonian formulation. We successfully circumvents this issue by treating the Ricci scalar as an independent field enforced via a Lagrange multiplier. This procedure effectively recasts the theory into a system with a Hamiltonian constraint that remains quadratic in the momenta, thereby preserving the applicability of the WKB approximation method developed in this tesis. For this, the analysis focuses principally on the spatially Flat FLRW Metric and proceeds through two distinct methodological stages. The first one motivated by the correspondence to maximally symmetric spacetimes often utilized in Euclidean treatments, this approach assumes that the Ricci scalar remains constant during the transition. This simplification reduces the governing dynamics from complex differential equations to algebraic constraints, allowing for the derivation of general analytical expressions for the transition probabilities. We treat with the power-law $f(R) = R^{1+n}$, this reveals a critical dependence on the exponent n. In the semiclassical contribution, the tension term exhibits a coefficient that changes sign at a specific critical value ($n = 2$), altering the decay rate behavior compared to the General Relativity limit. Crucially, while the first quantum correction merely modulates the probability amplitude, the second quantum correction introduces a behavior that fundamentally diverges from the classical prediction. As the scale factor approaches zero, the interplay between the semiclassical term and the second quantum correction forces the total probability to vanish at the origin and peak at a finite value. This confirms that the mechanism for avoiding the initial singularity, first observed in standard gravity, is robust and persists in modified gravity scenarios. Also, we compare the pure quadratic model (R^2) with the Starobinsky model ($R+\beta R^2$). The results indicate that while both models exhibit the same qualitative avoidance of the singularity via second-order corrections, the Starobinsky model is characterized by a more rapid decay of transition probabilities. This distinction is driven by additional model-dependent tension terms that arise specifically from the linear curvature contribution in the Starobinsky action.

The second approach, in order too validate that the avoidance of the singularity is a genuine physical prediction and not merely an artifact of the constant curvature approximation, we examine the full dynamical system where the Ricci scalar is allowed to vary. Focusing on the pure quadratic gravity case ($n = 1$), for which the probabilities are tractable, we fond that the logarithmic divergences that typically threaten the validity of the amplitude at the origin are shown to cancel naturally without the need for imposing auxiliary constraints on the potential, a significant improvement over the general realtivity and constant curvature cases. Most importantly, the full dynamical analysis recovers the exact qualitative behavior observed previously; the probability distribution vanishes at the singularity and attains its maximum at a non-zero scale factor. This provides strong evidence that the resolution of the initial singularity is a stable feature of the Lorentzian quantum cosmology framework, independent of the specific approximations applied to the Ricci scalar

We need to conclude candidly by identifying specific limitations regarding the Closed FLRW Metric. Unlike the flat case, the introduction of spatial curvature renders the constant Ricci scalar assumption mathematically inconsistent with a dynamic scale factor. Furthermore, the full differential equations for the closed universe in modified gravity do not admit analytical solutions even for simple models. Consequently, the explicit calculation of tension terms and transition probabilities for closed topologies in $f(R)$ gravity remains intractable within this specific analytical framework, marking a clear boundary for the current applicability of the method.

Let us remark, that in the Euclidean formalism the computation of the quantum corrections to the transition probabilities is troublesome. However, in the Lorentzian formalism we could compute such corrections in a fairly simple form by considering higher order terms in the semiclassical expansion. It will be interesting to investigate if some of the properties outlined in this article such as the avoidance of the initial singularity for the isotropic universe can also be encountered on the Euclidean formalism or if this represents a relevant departure from both approaches. Moreover, it could also be relevant to pursue a possible generalization of the current method to midisuperspace models. Finally, it is noteworthy that the results presented herein have provided insights into fundamental aspects. Despite the limitations inherent in the use of semiclassical approximations to the Wheeler-DeWitt equation for transition probabilities, we have succeeded in rigorously exploring critical issues such as the potential avoidance of the initial singularity in both isotropic and anisotropic universes, as well as the implications of modified gravity on these transitions.

Appendix A

Ordering ambiguities

As mentioned in chapters 1 and 2, the Wheeler-DeWitt equation is subject to operator ordering ambiguities arising from the promotion of conjugate momenta to operators, $\pi_M \to -i\hbar\frac{\delta}{\delta\Phi^M}$. In this section we examine an alternative ordering scheme to validate the suitability of the selected approach within the current framework.

A.1 Hermitian ordering

We proceed by employing the Hermitian ordering

$$G^{MN}(\Phi)\pi_M\pi_N \to \widehat{\pi}_M G^{MN}(\widehat{\Phi})\widehat{\pi}_N \tag{A.1}$$

Consequently, the WDW equation takes the form

$$\mathcal{H}\Psi(\Phi) = \left[-\frac{\hbar^2}{2}\frac{\delta}{\delta\Phi^M}G^{MN}(\Phi)\frac{\delta}{\delta\Phi^N} + \mathcal{V}[\Phi]\right]\Psi[\Phi] = 0 \tag{A.2}$$

Using the WKB ansatz, the equations for the first three orders in $\hbar$ are obtained as

$$\frac{1}{2}G^{MN}\frac{\delta S_0}{\delta\Phi^M}\frac{\delta S_0}{\delta\Phi^N} + \mathcal{V}[\Phi] = 0 \tag{A.3}$$

$$2G^{MN}\frac{\delta S_0}{\delta\Phi^M}\frac{\delta S_1}{\delta\Phi^N} = i\frac{\delta}{\delta\Phi^M}\left(G^{MN}\frac{\delta S_0}{\delta\Phi^N}\right) \tag{A.4}$$

$$2G^{MN}\frac{\delta S_0}{\delta\Phi^M}\frac{\delta S_2}{\delta\Phi^N} + G^{MN}\frac{\delta S_1}{\delta\Phi^M}\frac{\delta S_1}{\delta\Phi^N} = i\frac{\delta}{\delta\Phi^M}\left(G^{MN}\frac{\delta S_1}{\delta\Phi^N}\right) \tag{A.5}$$

It is observed that the first equation remains unmodified compared to (2.4); the changes are limited to the quantum corrections. We employ the definition of integral curves along classical trajectories [50, 51, 161]

$$C(s)\frac{d\Phi^M}{ds} = G^{MN}\frac{\delta S_0}{\delta\Phi^N} \tag{A.6}$$

and, by utilizing equation (A.3), the standard expression is found

$$S_0[\Phi] = -2\int^s \frac{ds'}{C(s')}\int_X \mathcal{V}\left[\Phi_{s'}\right] \tag{A.7}$$

Similarly, utilizing equation (A.4) yields

$$S_1[\Phi] = \frac{i}{2}\int^s \frac{ds'}{C(s')}\int_X \frac{\delta}{\delta\Phi^M}\left(G^{MN}\frac{\delta S_0}{\delta\Phi^N}\right) \tag{A.8}$$

The difference, compared to the alternative ordering, is that the metric tensor is now inside the functional derivative. Following the same procedure, the second correction term is found using equation (A.5)

$$S_2[\Phi] = \frac{i}{2}\int^s \frac{ds'}{C(s')}\int_X \frac{\delta}{\delta\Phi^M}\left(G^{MN}\frac{\delta S_1}{\delta\Phi^N}\right) - \frac{1}{2}\int^s \frac{ds'}{C(s')}\int_X G^{MN}\frac{\delta S_1}{\delta\Phi^M}\frac{\delta S_1}{\delta\Phi^N} \tag{A.9}$$

The difference here is that, once again, the metric is placed inside the functional derivative in the first term. Furthermore, since S_1 is modified, the second term will also change, despite maintaining the same functional form. Focusing on homogeneous metrics, it is straightforward to observe from (A.7) that

$$\frac{\delta S_0}{\delta\Phi^M} = -\frac{2\,\mathrm{Vol}(X)}{C(s)}\frac{\partial\mathcal{V}}{\partial\Phi^M}. \tag{A.10}$$

Assuming this functional derivative can be treated as a differentiable function for the second derivative, we propose

$$\frac{\delta^2 S_0}{\delta\Phi^M\delta\Phi^N} = -\frac{2\,\mathrm{Vol}(X)}{C(s)}\frac{\partial^2\mathcal{V}}{\partial\Phi^M\partial\Phi^N} \tag{A.11}$$

With this, the term within equation (A.4) can be written as

$$\frac{\delta}{\delta\Phi^M}\left(G^{MN}\frac{\delta S_0}{\delta\Phi^N}\right) = -\frac{2\,\mathrm{Vol}(X)}{C(s)}\frac{\partial}{\partial\Phi^M}\left(G^{MN}\frac{\partial\mathcal{V}}{\partial\Phi^N}\right). \tag{A.12}$$

The classical action is obtained simply as

$$S_0 = -2\,\mathrm{Vol}(X)\int^s \frac{\mathcal{V}}{C(s')}ds' \tag{A.13}$$

meaning there is no change in the classical action. Using the preceding result in equation (A.8) yields the first correction

$$S_1 = -i\,\mathrm{Vol}^2(X)\int^s \frac{ds'}{C^2(s')}\left(\nabla^2\mathcal{V} + \tilde{\nabla}G\cdot\tilde{\nabla}\mathcal{V}\right) \tag{A.14}$$

where we define

$$\tilde{\nabla}G\cdot\tilde{\nabla}\mathcal{V} = \frac{\partial G^{MN}}{\partial\Phi^M}\frac{\partial\mathcal{V}}{\partial\Phi^N}, \tag{A.15}$$

with the notation $\tilde{\nabla}G\cdot\tilde{\nabla}\mathcal{V}$ used to differentiate it from the dot product defined elsewhere in this thesis. Therefore, the change in the first correction is the inclusion of an extra term. Following the same procedure with the directional derivatives of S_1, we find for the second correction

$$\begin{aligned} S_2 =& \frac{\mathrm{Vol}^3(X)}{2}\int^s \frac{ds'}{C^3(s')}\left[\nabla^2\left(\nabla^2\mathcal{V}\right) + \nabla^2(\tilde{\nabla}G\cdot\tilde{\nabla}\mathcal{V}) + \tilde{\nabla}G\cdot\tilde{\nabla}\left(\nabla^2\mathcal{V} + \tilde{\nabla}G\cdot\tilde{\nabla}\mathcal{V}\right)\right] \\ &+ \frac{\mathrm{Vol}^5(X)}{2}\int^s \frac{ds'}{C^5(s')}\left[\left[\nabla\left(\nabla^2\mathcal{V}\right)\right]^2 + 2\nabla\left(\nabla^2\mathcal{V}\right)\cdot\nabla(\tilde{\nabla}G\cdot\tilde{\nabla}\mathcal{V}) + [\nabla(\tilde{\nabla}G\cdot\tilde{\nabla}\mathcal{V})]^2\right] \end{aligned} \tag{A.16}$$

Hence, the change in the second correction is the inclusion of four new terms. With these expressions, we proceed with the method to calculate the contributions to the transition probabilities. The semiclassical contribution yields the same result as in (2.32)

$$\begin{aligned} \Gamma_0 =& -\frac{2\,\mathrm{Vol}(X)i}{\hbar}\left\{\int_{s_0}^{\bar{s}-\delta s}\frac{ds}{C(s)}\mathcal{V}\bigg|_{\phi=\phi_B} - \int_{s_0}^{s-\delta s}\frac{ds}{C(s)}\mathcal{V}\bigg|_{\phi=\phi_A}\right. \\ &\left. + \int_{\bar{s}-\delta s}^{\bar{s}+\delta s} ds\left[\frac{\mathcal{V}}{C(s)} - \frac{\mathcal{V}}{C(s)}\bigg|_{\phi=\phi_A}\right]\right\} \end{aligned} \tag{A.17}$$

The first correction is found in this case as

$$\begin{aligned}\Gamma_1 = \mathrm{Vol}^2(X)\Bigg[&\int_{s_0}^{\bar{s}-\delta s}\frac{ds}{C^2(s)}\left(\nabla^2\mathcal{V}+\tilde{\nabla}G\cdot\tilde{\nabla}\mathcal{V}\right)\Big|_{\phi=\phi_B}-\int_{s_0}^{\bar{s}-\delta s}\frac{ds}{C^2(s)}\left(\nabla^2\mathcal{V}+\tilde{\nabla}G\cdot\tilde{\nabla}\mathcal{V}\right)\Big|_{\phi=\phi_A}\\ &+\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}ds\frac{1}{C^2(s)}\left(\nabla^2\mathcal{V}+\tilde{\nabla}G\cdot\tilde{\nabla}\mathcal{V}-\left(\nabla^2\mathcal{V}+\tilde{\nabla}G\cdot\tilde{\nabla}\mathcal{V}\right)\Big|_{\phi=\phi_A}\right)\Bigg]\end{aligned} \tag{A.18}$$

Consequently, there is an additional term within the integrals that must be computed. Furthermore, if $\tilde{\nabla}G\cdot\tilde{\nabla}\mathcal{V}$ is non-zero or not proportional to $\nabla^2\mathcal{V}$, an extra tension term arises for the first correction. Finally, the second correction is found as

$$\begin{aligned}\Gamma_2 =\frac{i\hbar}{2}\Bigg\{&\int_{s_0}^{\bar{s}-\delta s}ds\frac{\mathrm{Vol}^3(X)}{C^3(s)}\left[\nabla^2\left(\nabla^2\mathcal{V}\right)+\nabla^2(\tilde{\nabla}G\cdot\tilde{\nabla}\mathcal{V})+\tilde{\nabla}G\cdot\tilde{\nabla}\left(\nabla^2\mathcal{V}+\tilde{\nabla}G\cdot\tilde{\nabla}\mathcal{V}\right)\right]\Big|_{\phi=\phi_B}\\ &+\int_{s_0}^{\bar{s}-\delta s}ds\frac{\mathrm{Vol}^5(X)}{C^5(s)}\left[\left[\nabla\left(\nabla^2\mathcal{V}\right)\right]^2+2\nabla\left(\nabla^2\mathcal{V}\right)\cdot\nabla(\tilde{\nabla}G\cdot\tilde{\nabla}\mathcal{V})+[\nabla(\tilde{\nabla}G\cdot\tilde{\nabla}\mathcal{V})]^2\right]\Big|_{\phi=\phi_B}\\ &-\int_{s_0}^{\bar{s}-\delta s}ds\frac{\mathrm{Vol}^3(X)}{C^3(s)}\left[\nabla^2\left(\nabla^2\mathcal{V}\right)+\nabla^2(\tilde{\nabla}G\cdot\tilde{\nabla}\mathcal{V})+\tilde{\nabla}G\cdot\tilde{\nabla}\left(\nabla^2\mathcal{V}+\tilde{\nabla}G\cdot\tilde{\nabla}\mathcal{V}\right)\right]\Big|_{\phi=\phi_A}\\ &-\int_{s_0}^{\bar{s}-\delta s}ds\frac{\mathrm{Vol}^5(X)}{C^5(s)}\left[\left[\nabla\left(\nabla^2\mathcal{V}\right)\right]^2+2\nabla\left(\nabla^2\mathcal{V}\right)\cdot\nabla(\tilde{\nabla}G\cdot\tilde{\nabla}\mathcal{V})+[\nabla(\tilde{\nabla}G\cdot\tilde{\nabla}\mathcal{V})]^2\right]\Big|_{\phi=\phi_A}\\ &+\int_{\bar{s}-\delta_s}^{\bar{s}+\delta_s}ds\frac{\mathrm{Vol}^3(X)}{C^3(s)}\Big(\nabla^2\left(\nabla^2\mathcal{V}\right)+\nabla^2(\tilde{\nabla}G\cdot\tilde{\nabla}\mathcal{V})+\tilde{\nabla}G\cdot\tilde{\nabla}\left(\nabla^2\mathcal{V}+\tilde{\nabla}G\cdot\tilde{\nabla}\mathcal{V}\right)\\ &-\left[\nabla^2\left(\nabla^2\mathcal{V}\right)+\nabla^2(\tilde{\nabla}G\cdot\tilde{\nabla}\mathcal{V})+\tilde{\nabla}G\cdot\tilde{\nabla}\left(\nabla^2\mathcal{V}+\tilde{\nabla}G\cdot\tilde{\nabla}\mathcal{V}\right)\right]\Big|_{\phi=\phi_A}\Big)\\ &+\int_{\bar{s}-\delta_s}^{\bar{s}+\delta_s}ds\frac{\mathrm{Vol}^5(x)}{C^5(s)}\Big(\left[\nabla\left(\nabla^2\mathcal{V}\right)\right]^2+2\nabla\left(\nabla^2\mathcal{V}\right)\cdot\nabla(\tilde{\nabla}G\cdot\tilde{\nabla}\mathcal{V})+[\nabla(\tilde{\nabla}G\cdot\tilde{\nabla}\mathcal{V})]^2\\ &-\left[\left[\nabla\left(\nabla^2\mathcal{V}\right)\right]^2+2\nabla\left(\nabla^2\mathcal{V}\right)\cdot\nabla(\tilde{\nabla}G\cdot\tilde{\nabla}\mathcal{V})+[\nabla(\tilde{\nabla}G\cdot\tilde{\nabla}\mathcal{V})]^2\right]\Big|^2_{\phi=\phi_A}\Big)\Bigg\}.\end{aligned} \tag{A.19}$$

Therefore, there are several extra terms in the integrals; with the ordering choosen in (2.1), only the first term in each line appears. Furthermore, if all these terms are distinct, they will lead to various additional tension terms. We now proceed to perform the explicit calculations for the simplest metrics.

A.2 Flat FLRW Metric

For the flat FLRW metric, using equation (A.8) for the first correction yields

$$\Gamma_1 = \mathrm{Vol}(X)\left(\frac{V_B^{(2)}}{V_B}-\frac{V_A^{(2)}}{V_A}\right)\ln a\Big|_0^{\bar{a}}+\frac{\mathrm{Vol}(X)}{2}T_1, \tag{A.20}$$

which is the identical expression obtained with the alternative ordering. Specifically, the first term is eliminated by imposing the same condition on the second derivative of the potential. The only distinction lies in the definition of the tension term, which in this case is

$$\mathrm{Vol}(X)T_1 = \mathrm{Vol}^2(X)\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{ds}{C^2(s)}\left[V^{(2)}-\frac{V}{2}-\left(V_A^{(2)}-\frac{V_A}{2}\right)\Big|_{\phi=\phi_A}\right], \tag{A.21}$$

whereas in the previous ordering it was defined as

$$\mathrm{Vol}(X)T_1 = \mathrm{Vol}^2(X)\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{ds}{C^2(s)}\left[V^{(2)}-V-\left(V_A^{(2)}-V_A\right)\Big|_{\phi=\phi_A}\right]. \tag{A.22}$$

Consequently, the sole difference is that the tension possesses a distinct value; however, it remains a constant, thereby not modifying the general form of the curve, and the first correction continues to be merely a constant. Following the same procedure for equation (A.19), the second correction for this case is obtained as

$$\Gamma_2 = \pm\frac{i\hbar\,\mathrm{Vol}(X)}{2}\left(W_B - W_A\right)\frac{1}{3a^3}\,\Big|_{a_0}^{\bar{a}} + \frac{\mathrm{Vol}(X)\hbar}{\bar{a}^3}T_2, \tag{A.23}$$

which maintains the same general form. The difference arises in the definition of W, which in this instance is

$$W = \frac{\frac{V^{(2)}}{2} - V^{(4)}}{\sqrt{3}V^{3/2}} - \frac{\left(V^{(3)}\right)^2}{3\sqrt{3}V^{5/2}}, \tag{A.24}$$

while in the prior case it was defined as

$$W = \frac{V^{(2)} - V^{(4)}}{\sqrt{3}V^{3/2}} - \frac{\left(V^{(3)}\right)^2}{3\sqrt{3}V^{5/2}}. \tag{A.25}$$

Thus, the only difference lies in the term involving the second derivative. Therefore, imposing the condition $W_A = W_B$ to eliminate the divergence will lead to a slightly different constraint in each case. Similarly, the function utilized to define the tension T_2 in this ordering is

$$V^{(4)} - \frac{V^{(2)}}{2} + \left(V^{(3)}\right)^2, \tag{A.26}$$

whereas in the previous case it was

$$V^{(4)} - V^{(2)} + \left(V^{(3)}\right)^2. \tag{A.27}$$

Therefore, the constants are once again different. Consequently, this ordering does not alter the mechanism by which the singularity is eliminated; that is, it continues to be governed by the tension term with a dependence on $\bar{a}^{-3}$. Only the value of this constant and the condition for the higher derivatives of the potential are changed.

A.3 Closed FLRW Metric

We now consider the FLRW metric with positive curvature, which is of greater relevance for comparison with the Euclidean method. In this case, using equation (A.8), the first correction takes the form

$$\Gamma_1 = \pi^2\left[\left(\frac{V_B^{(2)}}{V_B} - 1\right)\ln\left(1 - V_B\bar{a}^2\right) - \left(\frac{V_A^{(2)}}{V_A} - 1\right)\ln\left(1 - V_A\bar{a}^2\right)\right] + 2\pi^2 T_1, \tag{A.28}$$

which is the same expression as obtained in the previous ordering. Once again, the only difference lies in the definition of the tension term, as the function used in this case is

$$V^{(2)} - \frac{V}{2}, \tag{A.29}$$

while in the previous ordering it was

$$V^{(2)} - V. \tag{A.30}$$

Thus, the tension terms are constants but have different values. Following the procedure and utilizing equation (A.19), the second correction in this case is obtained as

$$\begin{aligned}\Gamma_2 = \pm\pi^2\hbar \Bigg\{ &\left(V_B^{(4)} - \frac{V_B^{(2)}}{2}\right) F\left(V_B, a\right)\Bigg|_{a_0}^{\bar{a}} - \left(V_A^{(4)} - \frac{V_A^{(2)}}{2}\right) F\left(V_A, a\right)\Bigg|_{a_0}^{\bar{a}} \\ &- \left[\left(V_B^{(3)}\right)^2 G\left(V_B, a\right)\Bigg|_{a_0}^{\bar{a}} - \left(V_A^{(3)}\right)^2 G\left(V_A, a\right)\Bigg|_{a_0}^{\bar{a}}\right] + \frac{2}{3}\left[F_2\left(V_B, a\right)\big|_{a_0}^{\bar{a}} - F_2\left(V_A, a\right)\big|_{a_0}^{\bar{a}}\right] \\ &+\frac{1}{6}\left[G_2\left(V_B, a\right)\big|_{a_0}^{\bar{a}} - G_2\left(V_A, a\right)\big|_{a_0}^{\bar{a}}\right]\Bigg\} + \frac{2\pi^2\hbar}{\bar{a}^3} T_2.\end{aligned} \tag{A.31}$$

where the function used to define the tension term is again

$$V^{(4)} - \frac{V^{(2)}}{2} + \left(V^{(3)}\right)^2, \tag{A.32}$$

which differs from the previous ordering by the factor of 1/2. However, in this instance, two new functions appear in the result, defined by

$$\begin{aligned}F_2(V, a) &= \int \frac{\left(1 - a^2 V/3\right)^{1/2}}{a^3\left(1 - a^2 V\right)^2} \\ &= \frac{1}{12}\left[\frac{2\left(1 - 2Va^2\right)\sqrt{9 - 3Va^2} + 9\sqrt{6}V \operatorname{arctanh}\left(\frac{\sqrt{3 - Va^2}}{\sqrt{2}}\right)}{\sqrt{2}} - 22V \operatorname{arctanh}\sqrt{1 - \frac{Va^2}{3}}\right]\end{aligned} \tag{A.33}$$

$$\begin{aligned}G_2(V, a) = \int \frac{\left(1 - a^2 V/3\right)^{3/2}}{a^3\left(1 - a^2 V\right)^4} &= \\ &= \frac{\sqrt{9 - 3Va^2}\left(144 - 999Va^2 + 1378V^2a^4 - 555V^3a^6\right)}{864a^2\left(-1 + Va^2\right)^3} \\ &+ \frac{823V}{96\sqrt{6}} \operatorname{arctanh}\left(\frac{\sqrt{3 - Va^2}}{\sqrt{2}}\right) - \frac{7V}{2} \operatorname{arctanh}\sqrt{1 - \frac{Va^2}{3}}\end{aligned} \tag{A.34}$$

We now proceed to explore the conditions under which $a_0 = 0$ can be chosen. Analogously to the previous ordering, it is found that G presents no issue, and the divergence for F can be eliminated by choosing

$$V_B^{(4)} - \frac{V_B^{(2)}}{2} = V_A^{(4)} - \frac{V_A^{(2)}}{2}, \tag{A.35}$$

which is slightly different from the condition in the previous ordering due to the factor of 1/2. However, for the new terms, we have in this case that

$$\begin{aligned}\lim_{a\to 0} F_2(V, a) &= \frac{1}{12}\left[\frac{2}{a^2} + 9\sqrt{6} \operatorname{arctanh}\sqrt{\frac{3}{2}} - 22V \operatorname{arctanh}(1)\right], \\ \lim_{a\to 0} G_2(V, a) &= -\frac{1}{2a^2} + \frac{823V}{96\sqrt{6}} \operatorname{arctanh}\sqrt{\frac{3}{2}} - \frac{7V}{2} \operatorname{arctanh}(1).\end{aligned} \tag{A.36}$$

In both cases, the first term is a divergence that will cancel upon subtraction because it does not depend on the potential value, and the second term is simply a constant. However, the third term is a divergence that does depend on the potential, and in both instances, it can only be eliminated by taking

$$V_B = V_A, \tag{A.37}$$

which is impossible if a transition is desired. We thus conclude that this ordering does not allow access to the initial singularity for this metric. Therefore, the ordering utilized in the thesis is better in this regard.

Appendix B

Higher orders of semiclassical expansion

In this section, we present the calculation of the third quantum correction, corresponding to the fourth order in the semiclassical expansion. Furthermore, the specific behavior for FLRW metrics is shown.

Third quantum correction

Using the standard ordering chosen (2.1), substitution into the Wheeler-DeWitt equation for the fourth order of $\hbar$ yields to

$$G^{MN}\frac{\delta S_0}{\delta\Phi^M}\frac{\delta S_3}{\delta\Phi^N}=\frac{i}{2}G^{MN}\frac{\delta^2 S_2}{\delta\Phi^M\delta\Phi^N}-G^{MN}\frac{\delta S_1}{\delta\Phi^M}\frac{\delta S_2}{\delta\Phi^N} \tag{B.1}$$

Following the same treatment for the derivatives as in the section 2, the solution for S_3 is obtained as

$$\begin{aligned}S_3 =&\frac{\mathrm{Vol}^4(X)i}{4}\int_{a_0}^{\bar{s}-\delta s}\frac{ds}{C^4(s)}\nabla^6\mathcal{V}\\&+\frac{\mathrm{Vol}^6(X)i}{2}\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{ds}{C^6(s)}\left\{\frac{1}{2}\nabla^2\left[\nabla\left(\nabla^2\mathcal{V}\right)^2+\nabla\left(\nabla^2\mathcal{V}\right)\cdot\nabla\left(\nabla^4\mathcal{V}\right)\right]\right\}\\&+\frac{\mathrm{Vol}^8(X)i}{2}\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{ds}{C^8(s)}\nabla\left(\nabla^2\mathcal{V}\right)\cdot\nabla\left[\nabla\left(\nabla^2\mathcal{V}\right)^2\right]\end{aligned} \tag{B.2}$$

where the notation utilized is

$$\nabla^4\mathcal{V}=\nabla^2\left(\nabla^2\mathcal{V}\right),\quad \nabla^6\mathcal{V}=\nabla^2\left[\nabla^2\left(\nabla^2\mathcal{V}\right)\right]. \tag{B.3}$$

Consequently, the contribution to the transition probabilities is

$$
\begin{aligned}
\Gamma_3 =& -\frac{\mathrm{Vol}^4(X)\hbar^2}{4}\left[\int_0^{\bar{s}}\frac{ds}{C^4(s)}\nabla^6\mathcal{V}\Big|_{\phi=\phi_B}-\int_0^{\bar{s}}\frac{ds}{C^4(s)}\nabla^6\mathcal{V}\Big|_{\phi=\phi_A}\right]\\
&-\frac{\mathrm{Vol}^6(X)\hbar^2}{2}\left[\int_0^{\bar{s}}\frac{ds}{C^6(s)}\left(\frac{1}{2}\nabla^2\left[\nabla\left(\nabla^2\mathcal{V}\right)^2\right]+\nabla\left(\nabla^2\mathcal{V}\right)\cdot\nabla\left(\nabla^4\mathcal{V}\right)\right)\Big|_{\phi=\phi_B}\right.\\
&\left.-\int_0^{\bar{s}}\frac{ds}{C^6(s)}\left(\frac{1}{2}\nabla^2\left[\nabla\left(\nabla^2\mathcal{V}\right)^2\right]+\nabla\left(\nabla^2\mathcal{V}\right)\cdot\nabla\left(\nabla^4\mathcal{V}\right)\right)\Big|_{\phi=\phi_A}\right]\\
&-\frac{\mathrm{Vol}^8(X)\hbar^2}{2}\left[\int_0^{\bar{s}}\frac{ds}{C^8(s)}\nabla\left(\nabla^2\mathcal{V}\right)\cdot\nabla\left[\nabla\left(\nabla^2\mathcal{V}\right)^2\right]\Big|_{\phi=\phi_B}\right.\\
&\left.-\int_0^{\bar{s}}\frac{ds}{C^8(s)}\nabla\left(\nabla^2\mathcal{V}\right)\cdot\nabla\left[\nabla\left(\nabla^2\mathcal{V}\right)^2\right]\Big|_{\phi=\phi_A}\right]\\
&-\frac{\mathrm{Vol}^4(X)\hbar^2}{4}\left[\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{ds}{C^4(s)}\left(\nabla^6\mathcal{V}-\nabla^6\mathcal{V}\big|_{\phi=\phi_A}\right)\right]\\
&-\frac{\mathrm{Vol}^6(X)\hbar^2}{2}\left[\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{ds}{C^6(s)}\left\{\frac{1}{2}\nabla^2\left[\nabla\left(\nabla^2\mathcal{V}\right)^2\right]+\nabla\left(\nabla^2\mathcal{V}\right)\cdot\nabla\left(\nabla^4\mathcal{V}\right)\right.\right.\\
&\left.\left.-\left(\frac{1}{2}\nabla^2\left[\nabla\left(\nabla^2\mathcal{V}\right)^2\right]+\nabla\left(\nabla^2\mathcal{V}\right)\cdot\nabla\left(\nabla^4\mathcal{V}\right)\right)\Big|_{\phi=\phi_A}\right\}\right]\\
&-\frac{\mathrm{Vol}^8(X)\hbar^2}{2}\left[\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{ds}{C^8(s)}\left\{\nabla\left(\nabla^2\mathcal{V}\right)\cdot\nabla\left[\nabla\left(\nabla^2\mathcal{V}\right)^2\right]\right.\right.\\
&\left.\left.-\nabla\left(\nabla^2\mathcal{V}\right)\cdot\nabla\left[\nabla\left(\nabla^2\mathcal{V}\right)^2\right]\Big|_{\phi=\phi_A}\right\}\right]
\end{aligned}
\tag{B.4}
$$

We proceed to perform the calculation for the FLRW metrics, which constitute the simplest cases, in order to determine the behavior of this contribution.

B.1 Flat FLRW Metric

For the flat FLRW metric, it is found that

$$\nabla^6\mathcal{V}=\frac{1}{a^6}\left[V^{(6)}-3V^{(4)}-2V^{(2)}\right] \tag{B.5}$$

and the remaining terms are

$$
\begin{aligned}
&\frac{1}{2}\nabla^2\left[\nabla\left(\nabla^2\mathcal{V}\right)^2+\nabla\left(\nabla^2\mathcal{V}\right)\cdot\nabla\left(\nabla^4\mathcal{V}\right)\right]=\\
&=\frac{1}{a^6}\left[\left(V^{(4)}-V^{(2)}\right)^2+\left(V^{(3)}-V^{(1)}\right)\left(2V^{(5)}-3V^{(3)}+V^{(1)}\right)\right].
\end{aligned}
\tag{B.6}
$$

$$\nabla\left(\nabla^2\mathcal{V}\right)\cdot\nabla\left[\nabla\left(\nabla^2\mathcal{V}\right)^2\right]=\frac{2}{a^6}\left(V^{(3)}-V^{(1)}\right)^2\left(V^{(4)}-V^{(2)}\right). \tag{B.7}$$

With the preceding results, the complete calculation yields

$$\Gamma_3=\frac{\mathrm{Vol}(X)\hbar^2}{162}\left(U_B-U_A\right)\frac{1}{a^6}\Big|_{a_0}^{\bar{a}}+\mathrm{Vol}(X)\hbar^2\frac{T_3}{\bar{a}^6}, \tag{B.8}$$

where U is defined as

$$U = \frac{9}{4V^2}\left[V^{(6)} - 3V^{(4)} - 2V^{(2)}\right] + \frac{3}{2V^3}\left[\left(V^{(4)} - V^{(2)}\right)^2 + V^{(3)}\left(2V^{(5)} - 3V^{(3)}\right)\right] + \frac{1}{V^4}\left[V^{(3)}\right]^2\left(V^{(4)} - V^{(2)}\right). \tag{B.9}$$

From this result, we observe that in order to eliminate the divergence that appears when taking $a_0 = 0$, the condition $U_A = U_B$ must be imposed. Thus, the third correction is only a tension term with the same behavior as the second correction, but it is much less relevant in the infrared regime due to the power of $\bar{a}$ and the overall factor of $\hbar^2$. The expected result is therefore already obtained including only up to second order corrections.

B.2 Closed FLRW Metric

For this metric, the same results obtaining in (B.5), (B.6) and (B.7) are found, as the Laplacian is identical for both cases and the term differentiating them in $\mathcal{V}$ cancels out. Performing all calculations, the third correction is obtained as

$$\begin{aligned}\Gamma_3 =& \frac{\pi^2\hbar^2}{2}\left[\left(3V_B^{(4)} + 2V_B^{(2)} - V_B^{(6)}\right)F_{3,1}\left(V_B, a\right)\Big|_{a_0}^{\bar{a}}\right.\\ &\left. - \left(3V_A^{(4)} + 2V_A^{(2)} - V_A^{(6)}\right)F_{3,1}\left(V_A, a\right)\Big|_{a_0}^{\bar{a}}\right]\\ &+ \pi^2\hbar^2\left[\left\{\left(V_B^{(4)} - V_B^{(2)}\right)^2 + V_B^{(3)}\left(2V_B^{(5)} - 3V_B^{(3)}\right)\right\}F_{3,2}\left(V_B, a\right)\Big|_{a_0}^{\bar{a}}\right.\\ &\left. - \left\{\left(V_A^{(4)} - V_A^{(2)}\right)^2 + V_A^{(3)}\left(2V_A^{(5)} - 3V_A^{(3)}\right)\right\}F_{3,2}\left(V_A, a\right)\Big|_{a_0}^{\bar{a}}\right]\\ &+ 2\pi^2\hbar^2\left[\left(V_B^{(3)}\right)^2\left(V_B^{(2)} - V_B^{(4)}\right)F_{3,3}\left(V_B, a\right)\Big|_{a_0}^{\bar{a}}\right.\\ &\left. - \left(V_A^{(3)}\right)^2\left(V_A^{(2)} - V_A^{(4)}\right)F_{3,3}\left(V_A, a\right)\Big|_{a_0}^{\bar{a}}\right]\\ &+ 2\pi^2\hbar^2\frac{T_3}{\bar{a}^6},\end{aligned} \tag{B.10}$$

where the integral functions are defined as

$$F_{3,1}(V,a) = \int \frac{1 - \frac{V}{3}a^2}{a^3\left(1 - a^2V\right)^3}, \tag{B.11}$$

$$F_{3,2}(V,a) = \int \frac{\left(1 - \frac{V}{3}a^2\right)^2}{a\left(1 - a^2V\right)^5}, \tag{B.12}$$

$$F_{3,3}(V,a) = \int \frac{a\left(1 - \frac{V}{3}a^2\right)^3}{\left(1 - a^2V\right)^7}. \tag{B.13}$$

It is noted that the tension term exhibits the same dependence as in the preceding case, providing a mechanism to avoid the singularity, similar to the second quantum correction. The potential divergences that may occur when setting $a_0 = 0$ must now be checked. Upon evaluating the integrals, it is found that

$$F_{3,3}(V,a) = \frac{167 - 192Va^2 + 75V^2a^4 - 10V^3a^6}{1620V\left(1 - Va^2\right)^6}, \tag{B.14}$$

from which

$$\lim_{a\to 0} F_{3,3}(V,a) = \frac{167}{1620V}, \tag{B.15}$$

which presents no issues, as the result is constant. Similarly, it is found that

$$\begin{aligned} F_{3,2}(V,a) = {} & \ln a \\ & - \frac{1}{108\left(1-Va^2\right)^4}\left[-103 + 232Va^2 - 189V^2a^4 \right. \\ & \left. +54V^3a^6 + 54\left(1-Va^2\right)^4 \ln\left(1-Va^2\right)\right], \end{aligned} \tag{B.16}$$

which yields the limit

$$\lim_{a\to 0} F_{3,2}(V,a) = \ln a + \frac{103}{108}.$$

Therefore, to eliminate the logarithmic divergence, the condition

$$\left(V_B^{(4)} - V_B^{(2)}\right)^2 + V_B^{(3)}\left(2V_B^{(5)} - 3V_B^{(3)}\right) = \left(V_A^{(4)} - V_A^{(2)}\right)^2 + V_A^{(3)}\left(2V_A^{(5)} - 3V_A^{(3)}\right)$$

must be imposed. Finally, it is found that

$$F_{3,1}(V,a) = \frac{1}{3}\left[\frac{-3 + 12Va^2 - 8V^2a^4}{2a^2\left(1-Va^2\right)^2} + 8V\ln a - 4V\ln\left(1-Va^2\right)\right], \tag{B.17}$$

which has the limit

$$\lim_{a\to 0} F_{3,1}(V,a) = \frac{1}{3}\left[-\frac{3}{2a^2} + 8V\ln a\right]. \tag{B.18}$$

The divergence of the first term can be eliminated by choosing

$$3V_B^{(4)} + 2V_B^{(2)} - V_B^{(6)} = 3V_A^{(4)} + 2V_A^{(2)} - V_A^{(6)}. \tag{B.19}$$

However, by choosing this constraint to eliminate the first divergence, we are forced to choose $V_B = V_A$ to eliminate the second logarithmic divergence, which would preclude a transition. Thus, the third correction does not permit choosing $a_0 = 0$, even though the tension term exhibits the expected behavior. This indicates a potential limitation of the chosen ordering, as was observed in the case of the Hermitian ordering (See Appendix A).

Appendix C

Effects of a given factorization to the transition probabilities

In order to determine the effect of choosing a different factorization for the Hamiltonian constraint in the Bianchi III and flat FLRW metrics in $3+1$ dimensions, let us study a general factorization of the Hamiltonian of the Bianchi III metric (4.38) in the form

$$\begin{aligned} H =& N A^{-\gamma} B^{-\delta} C^{-\zeta} \Bigg[\frac{A^{\gamma+1} B^{\delta-1} C^{\zeta-1}}{4} \pi_A^2 + \frac{B^{\delta+1} A^{\gamma-1} C^{\zeta-1}}{4} \pi_B^2 + \frac{C^{\zeta+1} A^{\gamma-1} B^{\delta-1}}{4} \pi_C^2 \\ & - \frac{A^{\gamma} B^{\delta} C^{\zeta-1}}{2} \pi_A \pi_B - \frac{A^{\gamma} C^{\zeta} B^{\delta-1}}{2} \pi_A \pi_C - \frac{A^{\gamma-1} B^{\delta} C^{\zeta}}{2} \pi_B \pi_C + \frac{A^{\gamma-1} B^{\delta-1} C^{\zeta-1}}{2} \pi_\phi^2 \\ & + \alpha^2 A^{\gamma-1} B^{\delta+1} C^{\zeta+1} + V(\phi) A^{\gamma+1} B^{\delta+1} C^{\zeta+1} \Bigg] \simeq 0, \end{aligned} \tag{C.1}$$

where γ, δ and ζ are integers. We now consider the Hamiltonian constraint to be the terms within brackets, then, after identifying the metric and the corresponding $\mathcal{V}$ function we can proceed to relate the degrees of freedom of the metric when the scalar field is constant by employing eq. (**??**). In this case we obtain

$$\frac{dA}{dB} = \left(\frac{A}{B}\right) \frac{(\gamma-1-\delta-\zeta)V + \frac{\alpha^2}{A^2}(\gamma-3-\delta-\zeta)}{(\delta-1-\gamma-\zeta)V + \frac{\alpha^2}{A^2}(\delta+1-\gamma-\zeta)}, \tag{C.2}$$

and

$$\frac{dB}{dC} = \left(\frac{B}{C}\right) \frac{(\delta-1-\gamma-\zeta)V + \frac{\alpha^2}{A^2}(\delta+1-\gamma-\zeta)}{(\zeta-1-\gamma-\delta)V + \frac{\alpha^2}{A^2}(\zeta+1-\gamma-\delta)}. \tag{C.3}$$

The second relation is very difficult to solve because of the appearance of the A function. We can simplify this expression by choosing $\delta = \zeta$. Then, we obtain

$$B = b_0 C, \tag{C.4}$$

where b_0 is an integration constant that will be taken as 1. In the same way, it is found that

$$B = a_0 A^{\phi_1} \left[A^2 + \phi_2 \frac{\alpha^2}{V} \right]^{\phi_3}, \tag{C.5}$$

where a_0 is another integration constant that will be taken as 1 and

$$\phi_1 = \frac{1-\gamma}{\gamma-3-2\zeta}, \quad \phi_2 = \frac{\gamma-3-2\zeta}{\gamma-1-2\zeta}, \quad \phi_3 = \frac{2(\zeta+1)}{(2\zeta+1-\gamma)(2\zeta+3-\gamma)}. \tag{C.6}$$

Nevertheless, we want to obtain an isotropy limit that leads to the flat FLRW metric in order to correctly study the effect of anisotropy, that is we require $\lim_{\alpha=0} B = A$. This leads to the condition

$$\phi_1 + 2\phi_3 = 1, \tag{C.7}$$

which gives us the solution $\zeta = \gamma$. In this way, the most general factorization requires $\gamma = \zeta = \delta$. So the above definitions are simplified as

$$\phi_1 = \frac{\gamma - 1}{\gamma + 3}, \quad \phi_2 = \frac{\gamma + 3}{\gamma + 1}, \quad \phi_3 = \frac{2}{\gamma + 3}. \tag{C.8}$$

However, as we remarked in the main text the motivation to consider a different factorization is to have access to an initial singularity for the Bianchi III metric, that is that we can have $\lim_{A\to 0} B = 0$. We note from eq. (C.5) that this behaviour can be obtained by requiring that $\phi_1 > 0$, which leads to

$$\gamma > 1, \quad \text{or} \quad \gamma < -3. \tag{C.9}$$

Furthermore, the general form of the metric in minisuperspace is

$$\left(G^{MN}\right) = \frac{1}{2}\begin{pmatrix} A^{\gamma+1}(BC)^{\gamma-1} & -(AB)^{\gamma}C^{\gamma-1} & -(AC)^{\gamma}B^{\gamma-1} & 0 \\ -(AB)^{\gamma}C^{\gamma-1} & B^{\gamma+1}(AC)^{\gamma-1} & -(BC)^{\gamma}A^{\gamma-1} & 0 \\ -(AC)^{\gamma}B^{\gamma-1} & -(BC)^{\gamma}A^{\gamma-1} & C^{\gamma+1}(AB)^{\gamma-1} & 0 \\ 0 & 0 & 0 & 2(ABC)^{\gamma-1} \end{pmatrix} \tag{C.10}$$

and we can identify

$$\mathcal{V} = H(A,B,C) + F(A,B,C)V(\phi), \tag{C.11}$$

with

$$H(A,B,C) = \alpha^2 A^{\gamma-1}(BC)^{\gamma+1}, \quad F(A,B,C) = (ABC)^{\gamma+1}. \tag{C.12}$$

With these considerations, we can proceed to compute the transition probabilities with up to second quantum corrections using the general expressions (2.39), (2.41) and (2.42). However, we note that all the integrals on the three expressions will vanish in the limit $\bar{A} \to A_0 = 0$. Therefore, the behaviour of the transition probabilities in the singularity is dictated only by the tension terms. Thus, let us analyse the resulting tension terms due to the three contributions.

Following (2.39) the tension term for the semiclassical contribution takes the form

$$\frac{\mathrm{Vol}(X)}{\hbar}\bar{A}^{\frac{(\gamma+1)(3\gamma+1)}{\gamma+3}}\left[\bar{A}^2 + \frac{\gamma+3}{\gamma+1}\frac{\alpha^2}{V_B}\right]^{\frac{4(\gamma+1)}{\gamma+3}} T_0. \tag{C.13}$$

From this expression, we note that the important quantity to keep track, to study the behaviour in the initial singularity, is given by

$$\beta_0 = \frac{(\gamma+1)(3\gamma+1)}{\gamma+3}. \tag{C.14}$$

Furthermore, taking the limit $\alpha \to 0$ of (C.13) we are lead consistently to the tension term of the flat FLRW metric

$$\frac{\mathrm{Vol}(X)}{\hbar}\bar{a}^{3(\gamma+1)}T_0, \tag{C.15}$$

from where we note that relevant quantity is

$$\eta_0 = 3(\gamma+1). \tag{C.16}$$

In the same way, following (2.41) for the first quantum correction Γ_1, we obtain only one tension term written as

$$\mathrm{Vol}(X)\bar{A}^{\frac{2\gamma(3\gamma+1)}{\gamma+3}}\left[\bar{A}^2 + \frac{\gamma+3}{\gamma+1}\frac{\alpha^2}{V_B}\right]^{\frac{8\gamma}{\gamma+3}} T_1. \tag{C.17}$$

In the previous equation (C.17) we see that the relevant quantity to study the initial singularity is

$$\beta_1 = \frac{2\gamma(3\gamma+1)}{\gamma+3}. \tag{C.18}$$

One again, taking the limit $\alpha \to 0$, we obtain the corresponding tension term for the flat FLRW metric

$$\mathrm{Vol}(X)\bar{a}^{6\gamma}T_1, \tag{C.19}$$

where the relevant quantity is

$$\eta_1 = 6\gamma. \tag{C.20}$$

Finally, for the second quantum correction (2.42), we obtain only 3 different tension terms in the form

$$\begin{aligned}\mathrm{Vol}(X)\hbar\Bigg\{&\bar{A}^{\frac{9\gamma^2-1}{\gamma+3}}\left[\bar{A}^2+\frac{\gamma+3}{\gamma+1}\frac{\alpha^2}{V_B}\right]^{\frac{4(3\gamma-1)}{\gamma+3}}T_{2,1}+\bar{A}^{\frac{15\gamma^2-7}{\gamma+3}}\left[\bar{A}^2+\frac{\gamma+3}{\gamma+1}\frac{\alpha^2}{V_B}\right]^{\frac{4(5\gamma-1)}{\gamma+3}}T_{2,2}\\&+\bar{A}^{\frac{(5\gamma-1)(3\gamma+1)}{\gamma+3}}\left[\bar{A}^2+\frac{\gamma+3}{\gamma+1}\frac{\alpha^2}{V_B}\right]^{\frac{4(5\gamma-1)}{\gamma+3}}T_{2,3}\Bigg\}.\end{aligned} \tag{C.21}$$

Therefore, the relevant quantities for the second correction are

$$\beta_2 = \frac{9\gamma^2-1}{\gamma+3}, \qquad \beta_3 = \frac{15\gamma^2-7}{\gamma+3}, \qquad \beta_4 = \frac{(5\gamma-1)(3\gamma+1)}{\gamma+3}. \tag{C.22}$$

In this case, in order to obtain correctly the FLRW flat result, we need to take $\alpha \to 0$ and eliminate the second tension term since the functions depending on the scalar field vanish in this limit. Thus, we are led to

$$\mathrm{Vol}(X)a^{3(3\gamma-1)}T_{2,1}+\mathrm{Vol}(X)a^{3(5\gamma-1)}T_{2,3}, \tag{C.23}$$

from where we identify

$$\eta_2 = 3(3\gamma-1), \qquad \eta_3 = 3(5\gamma-1). \tag{C.24}$$

Therefore, the singularity will be the point of maximum probability for β_i and η_i positive, the general form of the probability distribution will not change for zero values of these parameters, whereas the singularity will be avoided if at least one of the β_i (for the Bianchi III metric) or one of the η_i (for the flat FLRW metric) is negative.

As asserted before we are interested in studying these behaviours for the regions where we can explore the initial singularity, that is $\gamma > 1$ or $\gamma < -3$. However, it can be shown that all β_i and η_i are positive for $\gamma > 1$ whereas all of these coefficients are negative for $\gamma < -3$. Since taking negative values for η_0 will change drastically our semiclassical results, we will not consider the region $\gamma < -3$. Therefore, focusing on $\gamma > 1$ we note that all coefficients are positive, thus, the singularity will remain as the point with maximum probability even after taking up to second quantum correction terms. Therefore, we conclude that the avoidance of the initial singularity by taking quantum corrections can only be performed in the isotropic universe.

Appendix D

General formalism with linear terms of the momenta

In this section, considering that the general method allows the inclusion of linear momentum terms, as shown in [53], we extend the calculation of quantum corrections to address this specific scenario. Let us consider the general Hamiltonian constraint

$$H = \frac{1}{2} G^{MN} \pi_M \pi_N + W^M(\Phi)\pi_M + \mathcal{V}(\Phi) \simeq 0. \tag{D.1}$$

We proceed with canonical quantization,

$$\pi_M \to -i\hbar \frac{\partial}{\partial \Phi^M}. \tag{D.2}$$

We note that the ordering ambiguities that may arise during quantization are implicitly contained within the vector W^M, which allows us to proceed with the quantization in this manner without loss of generality. We proceed as in all previous cases, namely by proposing the wave functional

$$\Psi = e^{\frac{i}{\hbar} S} \tag{D.3}$$

with $S = S_0 + \hbar S_1 + \hbar^2 S_2 + \hbar^3 S_3 + \mathcal{O}\left(\hbar^4\right)$. Consequently, from the WDW equation, the relations for the first four orders in $\hbar$ are found to be

$$\left(\frac{1}{2} G^{MN} \frac{\partial S_0}{\partial \Phi^M} + W^N\right) \frac{\partial S_0}{\partial \Phi^N} = -\mathcal{V}, \tag{D.4}$$

$$\left(G^{MN} \frac{\partial S_0}{\partial \Phi^M} + W^N\right) \frac{\partial S_1}{\partial \Phi^N} = \frac{i}{2} G^{MN} \frac{\partial^2 S_0}{\partial \Phi^M \partial \Phi^N}, \tag{D.5}$$

$$\left(G^{MN} \frac{\partial S_0}{\partial \Phi^M} + W^N\right) \frac{\partial S_2}{\partial \Phi^N} = \frac{i}{2} G^{MN} \frac{\partial^2 S_1}{\partial \Phi^M \partial \Phi^N} - \frac{1}{2} G^{MN} \frac{\partial S_1}{\partial \Phi^M} \frac{\partial S_1}{\partial \Phi^N}, \tag{D.6}$$

$$\left(G^{MN} \frac{\partial S_0}{\partial \Phi^M} + W^N\right) \frac{\partial S_3}{\partial \Phi^N} = \frac{i}{2} G^{MN} \frac{\partial^2 S_2}{\partial \Phi^M \partial \Phi^N} - G^{MN} \frac{\partial S_1}{\partial \Phi^M} \frac{\partial S_2}{\partial \Phi^N}. \tag{D.7}$$

Thus, in principle, the property is preserved that for each order in the semiclassical expansion, there is an independent equation derived from the WDW equation that allows for the calculation of the correction at the desired order. Furthermore, we again consider the integral curves defined as

$$C(s) \frac{d\Phi^M}{ds} = G^{MN} \frac{\partial S_0}{\partial \Phi^M}. \tag{D.8}$$

Using (D.4) and (D.8), it is found in this case that

$$S_0 = -2\int_X \int_s ds \left[\frac{\mathcal{V}}{C(s)} + W_M \frac{d\Phi^M}{ds}\right], \tag{D.9}$$

where $W_M = G_{MN}W^N$. Restricting to the homogeneous case, where the fields do not depend on the spatial variable, we can perform the variation of the classical action, whereby (D.8) leads to (what was already obtain in [53])

$$\begin{aligned}\frac{d\Phi^M}{ds} = &-\frac{2\,\mathrm{Vol}(X)}{C^2(s)}G^{MN}\frac{\partial \mathcal{V}}{\partial \Phi^N} - \frac{2\,\mathrm{Vol}(X)}{C(s)}\left[\left(G^{MN}G_{LP}\frac{\partial W^P}{\partial \Phi^N} - \frac{\partial W^M}{\partial \Phi^L}\right)\frac{d\Phi^L}{ds}\right.\\ &\left.+G^{MN}W^P\left(\frac{\partial G_{LP}}{\partial \Phi^N} - \frac{\partial G_{NP}}{\partial \Phi^L}\right)\frac{d\Phi^L}{ds}\right].\end{aligned} \tag{D.10}$$

On the other hand, manipulating (D.4) yields in this case

$$G_{MN}(\Phi)\frac{d\Phi^M}{ds}\frac{d\Phi^N}{ds} = -\frac{2}{C(s)}\left[\frac{\mathcal{V}(\Phi)}{C(s)} + W_P(\Phi)\frac{d\Phi^P}{ds}\right], \tag{D.11}$$

which can be written as a quadratic equation for $C(s)$ of the form

$$\left(G_{MN}(\Phi)\frac{d\Phi^M}{ds}\frac{d\Phi^N}{ds}\right)C^2(s) + 2W_M(\Phi)\frac{d\Phi^M}{ds}C(s) + 2\mathcal{V}(\Phi) = 0. \tag{D.12}$$

Thus, (D.10) and (D.12) form a system of equations for $\left\{\frac{d\Phi^M}{ds}, C(s)\right\}$, which in principle should be solvable, but must be addressed for specific cases. Writing as in the chapter 2

$$\mathcal{V}(\Phi) = H\left(\varphi^I\right) + F\left(\varphi^I\right)V(\phi), \tag{D.13}$$

we find in this instance for the semiclassical contribution

$$\begin{aligned}\Gamma_0 = -\frac{2i\,\mathrm{Vol}(X)}{\hbar}&\left[\int_0^{\bar{s}-\delta s} ds\left[\frac{\mathcal{V}}{C(s)} + W_M\frac{d\Phi^M}{ds}\right]\Bigg|_{\phi=\phi_B}\right.\\ &\left.-\int_0^{\bar{s}-\delta s} ds\left[\frac{\mathcal{V}}{C(s)} + W_M\frac{d\Phi^M}{ds}\right]\Bigg|_{\phi=\phi_A}\right]\\ &+\frac{\mathrm{Vol}(X)}{\hbar}F\Big|_{\bar{\Phi}}T_0\\ &-\frac{2i\,\mathrm{Vol}(X)}{\hbar}\int_{\bar{s}-\delta s}^{\bar{s}+\delta s} ds\left[W_M\frac{d\Phi^M}{ds} - W_M\frac{d\Phi^M}{ds}\Big|_{\phi=\phi_A}\right].\end{aligned} \tag{D.14}$$

To perform the first two integrals, the system of equations must be solved and the fields related, if possible, such that they can be written as integrals over only one of the spatial metric's degrees of freedom. Whether this is possible must be assessed for specific cases. For FLRW metrics, which possess only the scale factor, this should generally be feasible. On the other hand, the first tension term is the one that appears in the case without linear terms; however, the final term can only be interpreted as a tension term if it possesses the appropriate structure, which must be analyzed in each specific case.

For the first correction in the previous case, the following expressions were used

$$\frac{dS_1}{ds} = \int_X \frac{d\Phi^M}{ds}\frac{\delta S_1}{\delta \Phi^M} = \int_X \frac{1}{C(s)}G^{MN}\frac{\delta S_0}{\delta \Phi^M}\frac{\delta S_1}{\delta \Phi^N}. \tag{D.15}$$

Subsequently, equation (D.5) was used to relate the final term to second variational derivatives of S_0. However, we note from this equation that due to the presence of the vector W^M, this can no longer be done, as the term $\frac{\delta S_1}{\delta \Phi^M}$ would remain on the right-hand side. This same issue occurs in all other equations for all quantum corrections. Therefore, in this case, we cannot directly write the quantum corrections as integrals over the parameter s of known functions. Nevertheless, based on the previous results, we can assume that S_1 can be written in general as

$$S_1 = \int F_1(\Phi, s) ds, \tag{D.16}$$

from which

$$\frac{\delta S_1}{\delta \Phi^M} = \frac{\partial F_1}{\partial \Phi^M}. \tag{D.17}$$

Thus, the first correction is written as

$$\begin{aligned}\Gamma_1 = i & \left[\int_0^{\bar{s}-\delta s} F_1(\Phi, s)\Big|_{\phi=\phi_B} ds - \int_0^{\bar{s}-\delta s} F_1(\Phi, s)\Big|_{\phi=\phi_A} ds \right] \\ & + i \int_{\bar{s}-\delta s}^{\bar{s}+\delta s} \left(F_1(\Phi, s) - F_1(\Phi, s)|_{\phi=\phi_A} \right) ds,\end{aligned} \tag{D.18}$$

where the function F_1 must satisfy equation (D.5), which is written as a differential equation of the form

$$\left[C(s) \frac{d\Phi^M}{ds} + W^M \right] \frac{\partial F_1}{\partial \Phi^M} = \frac{i}{2} G^{MN} \frac{\delta^2 S_0}{\delta \Phi^M \delta \Phi^N}. \tag{D.19}$$

If the semiclassical contribution has already been calculated, all terms within the bracket and the term on the right-hand side are known. Furthermore, if the system of equations allows for the relating of the metric's degrees of freedom, this will be a partial differential equation involving only the terms $\frac{\partial F_1}{\partial \Phi^i}$ (with Φ^i being the independent degree of freedom from the metric) and $\frac{\partial F_1}{\partial \phi}$. We also note from (D.18) that if this occurs, the first two integrals can be converted into integrals over this metric degree of freedom without issue. Moreover, for the third integral to yield a tension term, it must be expressible in the form

$$F_1(\Phi, s) = f_1(\Phi) g_1(\phi) h_1(s) = f_1\left(\Phi^i\right) g_1(\phi) h_1(s), \tag{D.20}$$

as occurred in the previous cases. With this ansatz and under these conditions, there is, in principle, one way of solving the differential equation for certain cases. The same complications arise for the second and third corrections, for which we can propose in those cases

$$S_2 = \int F_2(\Phi, s) ds, \tag{D.21}$$

$$S_3 = \int F_3(\Phi, s) ds. \tag{D.22}$$

The contributions to the transition probabilities will then take the form

$$\begin{aligned}\Gamma_2 = & i\hbar \left[\int_0^{\bar{s}-\delta s} F_2(\Phi, s)\Big|_{\phi=\phi_B} ds - \int_0^{\bar{s}-\delta s} F_2(\Phi, s)\Big|_{\phi=\phi_A} ds \right] \\ & + i\hbar \int_{\bar{s}-\delta s}^{\bar{s}+\delta s} \left(F_2(\Phi, s) - F_2(\Phi, s)|_{\phi=\phi_A} \right) ds,\end{aligned} \tag{D.23}$$

$$
\begin{aligned}
\Gamma_3 =& i\hbar^2 \left[\int_0^{\bar{s}-\delta s} F_3(\Phi, s)\bigg|_{\phi=\phi_B} ds - \int_0^{\bar{s}-\delta s} F_3(\Phi, s)\bigg|_{\phi=\phi_A} ds \right] \\
&+ i\hbar^2 \int_{\bar{s}-\delta s}^{\bar{s}+\delta s} \left(F_3(\Phi, s) - F_3(\Phi, s)|_{\phi=\phi_A} \right) ds,
\end{aligned} \tag{D.24}
$$

where the functions F_2 and F_3 satisfy the partial differential equations

$$
\left[C(s)\frac{d\Phi^M}{ds} + W^M \right] \frac{\partial F_2}{\partial \Phi^M} = \frac{i}{2}\nabla^2 F_1 - \frac{1}{2}\left(\nabla F_1\right)^2, \tag{D.25}
$$

$$
\left[C(s)\frac{d\Phi^M}{ds} + W^M \right] \frac{\partial F_3}{\partial \Phi^M} = \frac{i}{2}\nabla^2 F_2 - \nabla F_1 \cdot \nabla F_2. \tag{D.26}
$$

In conclusion, although we may not have general expressions, we possess sufficient expressions to calculate the transition probabilities with quantum corrections to any order by analyzing specfic cases.

D.1 Laplace-Beltrami Operator

In order to consider at least one relevant scenario, the objective of this section is to study the transitions under a distinct operator ordering. The most relevant and straightforward ordering to implement involves quantization via the Laplace-Beltrami operator, which is expressed as

$$
G^{MN}\pi_M\pi_N \to \frac{1}{\sqrt{-G}}\frac{\delta}{\delta\Phi^M}\left(\sqrt{-G}G^{MN}\frac{\delta}{\delta\Phi^N}\right). \tag{D.27}
$$

To simplify the scenario, we shall consider the flat FLRW metric in 3+1 dimensions. The superspace metric is therefore diagonal (see chapter 4), with components

$$
G^{aa} = -\frac{1}{6a}, \quad G^{\phi\phi} = \frac{1}{a^3}, \tag{D.28}
$$

and furthermore,

$$
\sqrt{-G} = \sqrt{6}a^2. \tag{D.29}
$$

Consequently, upon quantization, we find that

$$
G^{MN}\pi_M\pi_N \to G^{MN}\frac{\delta}{\delta\Phi^M}\frac{\delta}{\delta\Phi^N} - \frac{1}{6a^2}\frac{\delta}{\delta a}. \tag{D.30}
$$

The first term is identical to the one obtained under the quantization studied thus far. The second term can be incorporated as a linear momentum term, corresponding to a superspace vector W^M given by

$$
W^a = -\frac{1}{6a^2}, \quad W^\phi = 0, \tag{D.31}
$$

which implies the covariant components are

$$
W_a = \frac{1}{a}, \quad W_\phi = 0. \tag{D.32}
$$

Using the general method with linear terms, it was previously found that the derivatives of the superspace fields are given by

$$
\begin{aligned}
\frac{d\Phi^M}{ds} =& -\frac{2\,\mathrm{Vol}(X)}{C^2(s)}G^{MN}\frac{\partial \mathcal{V}}{\partial \Phi^N} - \frac{2\,\mathrm{Vol}(X)}{C(s)}\Big[\Big(G^{MN}G_{LP} \quad \frac{\partial W^P}{\partial \Phi^N} - \frac{\partial W^M}{\partial \Phi^L}\Big)\frac{d\Phi^L}{ds} \\
&+ G^{MN}W^P\left(\frac{\partial G_{LP}}{\partial \Phi^N} - \frac{\partial G_{NP}}{\partial \Phi^L}\right)\frac{d\Phi^L}{ds}\Big],
\end{aligned} \tag{D.33}
$$

and the system of equations is complemented by the quadratic equation

$$\left(G_{MN}(\Phi)\frac{d\Phi^M}{ds}\frac{d\Phi^N}{ds}\right)C^2(s)+2W_M(\Phi)\frac{d\Phi^M}{ds}C(s)+2\mathcal{V}(\Phi)=0. \tag{D.34}$$

In the present case, this system simplifies considerably to

$$\frac{da}{ds}=\frac{\mathrm{Vol}(X)aV}{C^2(s)}, \tag{D.35}$$

$$\frac{d\phi}{ds}=-\frac{2\,\mathrm{Vol}(X)}{C^2(s)}V^{(1)}. \tag{D.36}$$

This simplification occurs because all terms on the right-hand side of (D.33), except for the first, vanish. This is due to the fact that only W^a is non-zero, the superspace metric is diagonal, and both the metric and W^a depend exclusively on the scale factor a. Since these conditions also hold for the closed FLRW metric, it is expected that the system of equations will also simplify considerably in that case.

For cases where the potential is constant, $C(s)$ must be found from the quadratic equation (D.34). In this context, the equation is written as

$$x^2\mp\frac{x}{3a^2}-\frac{a^2V}{3}=0,$$

where $x=\sqrt{\mathrm{Vol}(X)aV\frac{da}{ds}}$. This can be solved for $\frac{da}{ds}$, and subsequently $C(s)$ is found to be

$$C(s)=(\pm)_1\frac{6\,\mathrm{Vol}(X)a^3V}{(\pm)_1 1(\pm)_2\sqrt{1+12a^6V}}, \tag{D.37}$$

where $(\pm)_{1,2}$ denote unrelated sign ambiguities, distinguished by the subscript. The semiclassical contribution to the transition probability was previously found to be

$$\begin{aligned}\Gamma_0=&-\frac{2i\,\mathrm{Vol}(X)}{\hbar}\left[\int_0^{\bar{s}-\delta s}ds\left[\frac{\mathcal{V}}{C(s)}+W_M\frac{d\Phi^M}{ds}\right]\Bigg|_{\phi=\phi_B}\right.\\&\left.-\int_0^{\bar{s}-\delta s}ds\left[\frac{\mathcal{V}}{C(s)}+W_M\frac{d\Phi^M}{ds}\right]\Bigg|_{\phi=\phi_A}\right]\\&+\frac{\mathrm{Vol}(X)}{\hbar}F\Big|_{\bar{\Phi}}T_0-\frac{2i\,\mathrm{Vol}(X)}{\hbar}\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}ds\left[W_M\frac{d\Phi^M}{ds}-W_M\frac{d\Phi^M}{ds}\Big|_{\phi=\phi_A}\right].\end{aligned} \tag{D.38}$$

Substituting these results into the semiclassical expression, we find

$$\begin{aligned}\Gamma_0=(\mp)_1\frac{12i\,\mathrm{Vol}(X)}{\hbar}&\left[V_B\int_0^{\bar{a}}\frac{a^5}{(\pm)_1 1(\pm)_2\sqrt{1+12a^6V_B}}da\right.\\&\left.-V_A\int_0^{\bar{a}}\frac{a^5}{(\pm)_1 1(\pm)_2\sqrt{1+12a^6V_A}}da\right]\\&+\frac{\mathrm{Vol}(X)}{\hbar}\left[\bar{a}^3T_0+T_1\right].\end{aligned} \tag{D.39}$$

It is observed that the behavior of the new tension term T_1 is analogous to that which appeared in the first quantum correction of the ordering considered in chapter 2. We also note that due to the global factor of i in the first integrals, it is possible that these terms only contribute for negative potentials, as was the case in the prior ordering. In such a scenario, the integrals must be evaluated by selecting the appropriate signs to determine the effect. Within the general method, it was proposed that the first correction can be written as

$$\begin{aligned}\Gamma_1 = i &\left[\int_0^{\bar{s}-\delta s} F_1(\Phi, s)\Big|_{\phi=\phi_B} ds - \int_0^{\bar{s}-\delta s} F_1(\Phi, s)\Big|_{\phi=\phi_A} ds \right] \\ &+ i \int_{\bar{s}-\delta s}^{\bar{s}+\delta s} \Big(F_1(\Phi, s) - F_1(\Phi, s)|_{\phi=\phi_A} \Big)\, ds,\end{aligned} \tag{D.40}$$

where F_1 satisfies the differential equation

$$\left[C(s) \frac{d\Phi^M}{ds} + W^M \right] \frac{\partial F_1}{\partial \Phi^M} = \frac{i}{2} G^{MN} \frac{\delta^2 S_0}{\delta \Phi^M \delta \Phi^N}. \tag{D.41}$$

Furthermore, the classical action S_0 is given by

$$S_0 = -2\,\mathrm{Vol}(X) \int ds \left[\frac{\mathcal{V}}{C(s)} + W_M \frac{d\Phi^M}{ds} \right]. \tag{D.42}$$

For the flat FLRW metric, one finds

$$\frac{\mathcal{V}}{C(s)} + W_M \frac{d\Phi^M}{ds} = \frac{a^3 V}{C(s)} + \frac{\mathrm{Vol}(X)}{C^2(s)} V. \tag{D.43}$$

Consequently, the differential equation (D.41) takes the specific form

$$\left[\frac{\mathrm{Vol}(X)}{C(s)} aV - \frac{1}{6a^2} \right] \frac{\partial F_1}{\partial a} - \frac{2\,\mathrm{Vol}(X)}{C(s)} V^{(1)} \frac{\partial F_1}{\partial \phi} = \frac{i}{2} \left[\frac{V^{(2)} - V}{C(s)} + \frac{\mathrm{Vol}(X)}{a^3 C^2(s)} V^{(2)} \right]. \tag{D.44}$$

It is observed that, due to the presence of the first term within the brackets of the partial derivative, this equation proves resistant to solution via the method of separation of variables. Consequently, while a comprehensive search for potential solutions is warranted, such an analysis lies beyond the scope of the present work. Despite this, the Lorentzian framework based on the Wheeler-DeWitt equation proves to be a robust approach for addressing distinct operator orderings in vacuum transitions analysis.

Appendix E

Bianchi III metric in $f(R)$ gravity

In this section, with the aim of incorporating anisotropy into the framework of $f(R)$ gravity, we examine the Bianchi Type III metric, which describes homogeneous yet anisotropic universes. In a local coordinate system, the line element is given by

$$ds^2 = -N^2(t)dt^2 + A^2(t)dx^2 + B^2(t)e^{-2\alpha x}dy^2 + C^2(t)dz^2, \tag{E.1}$$

where $\alpha \neq 0$ is a constant parameterizing the degree of anisotropy. Assuming, as in previous sections, a homogeneous scalar field coupled to modified gravity within this metric background, the Ricci scalar is calculated as

$$\begin{aligned} R =& \frac{2}{A^2BCN^3}\{A[AN\dot{B}\dot{C} + C(N\dot{A}\dot{B} - A\dot{B}\dot{N} + AN\ddot{B})] \\ &+ B\left[-C\left(\alpha^2N^3 + A\dot{A}\dot{N} - AN\ddot{A}\right)\right. \\ &+ A(N\dot{A}\dot{C} - A\dot{C}\dot{N} + AN\ddot{C})]\}. \end{aligned} \tag{E.2}$$

Consequently, the Lagrangian assumes the form

$$\begin{aligned} \mathcal{L} =& \frac{NABC}{2}(f - f_R R) - \alpha^2 f_R \frac{BCN}{A} - NABCV(\phi) + \frac{ABC}{2N}\dot{\phi}^2 \\ &- \frac{f_{RR}}{N}\dot{R}(\dot{A}BC + A\dot{B}C + AB\dot{C}) - \frac{f_R}{N}(\dot{A}B\dot{C} + \dot{A}\dot{B}C + A\dot{B}\dot{C}), \end{aligned} \tag{E.3}$$

from which the canonical momenta are derived as

$$\begin{aligned} \pi_N &= \frac{\partial L}{\partial \dot{N}} = 0, \\ \pi_A &= \frac{\partial L}{\partial \dot{A}} = -\frac{f_{RR}}{N}\dot{R}BC - \frac{f_R}{N}(B\dot{C} + \dot{B}C), \\ \pi_B &= \frac{\partial L}{\partial \dot{B}} = -\frac{f_{RR}}{N}\dot{R}AC - \frac{f_R}{N}(\dot{A}C + A\dot{C}), \\ \pi_C &= \frac{\partial L}{\partial \dot{C}} = -\frac{f_{RR}}{N}\dot{R}AB - \frac{f_R}{N}(\dot{A}B + A\dot{B}), \\ \pi_R &= \frac{\partial L}{\partial \dot{R}} = -\frac{f_{RR}}{N}(\dot{A}BC + A\dot{B}C + AB\dot{C}), \\ \pi_\phi &= \frac{\partial L}{\partial \dot{\phi}} = \frac{ABC}{N}\dot{\phi} \Rightarrow \dot{\phi} = \frac{\pi_\phi N}{ABC}. \end{aligned} \tag{E.4}$$

Based on the foregoing, the resulting Hamiltonian is

$$
\begin{aligned}
H = N\Bigg[&\frac{1}{3ABC}\frac{1}{f_R}\left(A^2\pi_A^2 + B^2\pi_B^2 + C^2\pi_C^2\right) + \frac{1}{3ABC}\frac{f_R}{f_{RR}^2}\pi_R^2 + \frac{1}{2ABC}\pi_\phi^2 \\
&- \frac{1}{3C}\frac{1}{f_R}\pi_A\pi_B - \frac{1}{3B}\frac{1}{f_R}\pi_A\pi_C - \frac{1}{3A}\frac{1}{f_R}\pi_B\pi_C \\
&- \frac{1}{3BC}\frac{1}{f_{RR}}\pi_A\pi_R - \frac{1}{3AC}\frac{1}{f_{RR}}\pi_B\pi_R - \frac{1}{3AB}\frac{1}{f_{RR}}\pi_C\pi_R \\
&+\frac{1}{2}ABC\left(Rf_R - f\right) + ABCV(\phi) + \alpha^2\frac{BC}{A}f_R\Bigg] \approx 0,
\end{aligned}
\tag{E.5}
$$

which satisfies the general form of the Hamiltonian constraint

$$
H = N\left(\frac{1}{2}G^{MN}\pi_M\pi_N + \mathcal{V}\right). \tag{E.6}
$$

From this, we identify the components of the metric

$$
G^{MN} = \begin{pmatrix}
\frac{2A}{3BCf_R} & -\frac{1}{3Cf_R} & -\frac{1}{3Bf_R} & -\frac{1}{3BCf_{RR}} & 0 \\
-\frac{1}{3Cf_R} & \frac{2B}{3ACf_R} & -\frac{1}{3Af_R} & -\frac{1}{3ACf_{RR}} & 0 \\
-\frac{1}{3Bf_R} & -\frac{1}{3Af_R} & \frac{2C}{3ABf_R} & -\frac{1}{3ABf_{RR}} & 0 \\
-\frac{1}{3BCf_{RR}} & -\frac{1}{3ACf_{RR}} & -\frac{1}{3ABf_{RR}} & \frac{2f_R}{3ABCf_{RR}^2} & 0 \\
0 & 0 & 0 & 0 & \frac{1}{ABC}
\end{pmatrix}, \tag{E.7}
$$

and the function

$$
\mathcal{V} = \frac{1}{2}ABC(f_R R - f) + \frac{\alpha^2 BCf_R}{A} + ABCV(\phi). \tag{E.8}
$$

At this stage, we possess all necessary elements to apply the general formalism. The resulting solutions are

$$
C^2 = \frac{2\,\mathrm{Vol}(X)\left[3A^2(f-2V)\left(A^2R+2\alpha^2\right) - 2\left(A^4R^2+2A^2R\alpha^2-8\alpha^4\right)f_R\right]}{3A^4(f-2V) - 3\left(A^4R+2A^2\alpha^2\right)f_R}, \tag{E.9}
$$

$$
\frac{dA}{ds} = -\frac{A\left(A^2R+10\alpha^2\right)\left[-A^2(f-2V)+\left(A^2R+2\alpha^2\right)f_R\right]}{2\,\mathrm{Vol}(X)\left[3A^2(f-2V)\left(A^2R+2\alpha^2\right)-2\left(A^4R^2+2A^2R\alpha^2-8\alpha^4\right)f_R\right]}, \tag{E.10}
$$

the relationships between the metric variables and the additional degree of freedom R result

$$
\begin{aligned}
\frac{dA}{dR} &= \frac{A\left(A^2R+10\alpha^2\right)f_{RR}}{-3A^2f+6A^2V+\left(A^2R-2\alpha^2\right)f_R}, \\
\frac{dB}{dR} &= \frac{B\left(A^2R-2\alpha^2\right)f_{RR}}{-3A^2f+6A^2V+\left(A^2R-2\alpha^2\right)f_R}, \\
\frac{dC}{dR} &= \frac{C\left(A^2R-2\alpha^2\right)f_{RR}}{-3A^2f+6A^2V+\left(A^2R-2\alpha^2\right)f_R},
\end{aligned}
\tag{E.11}
$$

and the relations between the metric variables result in

$$
\begin{aligned}
\frac{dA}{dB} &= \frac{A^3R+10A\alpha^2}{A^2BR-2B\alpha^2}, \\
\frac{dA}{dC} &= \frac{A^3R+10A\alpha^2}{A^2CR-2C\alpha^2}, \\
\frac{dB}{dC} &= \frac{B}{C}.
\end{aligned}
\tag{E.12}
$$

The semiclassical contribution can be expressed as

$$\begin{aligned}
&\frac{ds}{C(s)}\mathcal{V} = -\frac{BC}{\sqrt{2}\left(A^4R+10\alpha^2A^2\right)}\{3\left(A^4R+2\alpha^2A^2\right)f\\
&-2\left[-3A^4V'^2+\left(-8\alpha^4+A^4R^2+2\alpha^2A^2R\right)f_R+3V\left(A^4R+2\alpha^2A^2\right)\right]\}\times\\
&\times\sqrt{\frac{-3A^4f+6A^4V+3A^2\left(2\alpha^2+A^2R\right)f_R}{2\left[-3A^4V'^2+\left(-8\alpha^4+A^4R^2+2\alpha^2A^2R\right)f_R+3V\left(A^4R+2\alpha^2A^2\right)\right]-3\left(A^4R+2\alpha^2A^2\right)f}},
\end{aligned} \tag{E.13}$$

yielding

$$\begin{aligned}
\Gamma_0 = &-\frac{2\,\mathrm{Vol}(X)i}{\hbar}\{\int_0^{\bar{s}-\delta s}\frac{ds}{C(s)}\mathcal{V}\bigg|_{\phi=\phi_B}-\int_0^{s-\delta s}\frac{ds}{C(s)}\mathcal{V}\bigg|_{\phi=\phi_A}\}\\
&-\frac{2\,\mathrm{Vol}(X)i}{\hbar}\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{ds}{C(s)}ABC\left(V-V_A\right)\\
&-\frac{2\,\mathrm{Vol}(X)i}{\hbar}\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{ds}{C(s)}\frac{ABC}{2}\left[\left(f_RR-f\right)-\left(f_RR-f\right)|_{\phi_A}\right]\\
&-\frac{2\,\mathrm{Vol}(X)i}{\hbar}\int_{s-\delta s}^{\bar{s}+\delta s}\frac{ds}{C(s)}\frac{BC}{A}\alpha^2\left(f_R-f_R|_{\phi_A}\right).
\end{aligned} \tag{E.14}$$

Proceeding to the first quantum correction, we obtain

$$\begin{aligned}
\nabla^2\mathcal{V} = \frac{1}{3}\Bigg(&-6R+\frac{4\alpha^2}{A^2}+\frac{3f}{f_R}-\frac{6V}{f_R}+\frac{f_R}{f_{RR}}+3V^{(2)}\\
&+\frac{Rf_Rf_{RRR}}{f_{RR}^2}+\frac{2\alpha^2f_Rf_{RRR}}{A^2f_{RR}^2}\Bigg).
\end{aligned} \tag{E.15}$$

In this way, we can write

$$\begin{aligned}
\frac{ds}{C^2(s)}\nabla^2\mathcal{V} = &\frac{1}{A\left(A^2R+10\alpha^2\right)f_Rf_{RR}^2}\Big\{3A^2(f-2V)f_{RR}^2\\
&+f_Rf_{RR}^2\left(-6A^2R+4\alpha^2+3A^2V^{(2)}\right)\\
&+f_R^2\left[A^2f_{RR}+\left(A^2R+2\alpha^2\right)f_{RRR}\right]\Big\}.
\end{aligned} \tag{E.16}$$

Thus, Γ_1 is given by

$$\begin{aligned}
\Gamma_1 = &\,\mathrm{Vol}(X)\left[\int_0^{\bar{s}-\delta s}\frac{ds}{C^2(s)}\nabla^2\mathcal{V}\bigg|_{\phi=\phi_B}-\int_0^{\bar{s}-\delta s}\frac{ds}{C^2(s)}\nabla^2\mathcal{V}\bigg|_{\phi=\phi_A}\right]\\
&+\mathrm{Vol}^2(X)\int_{s-\delta s}^{\bar{s}+\delta s}\frac{ds}{C^2(s)}\left(V^{(2)}-V_A^{(2)}\right)\\
&+\mathrm{Vol}^2(X)\int_{\bar{s}-\delta s}^{\bar{s}+\delta s}\frac{ds}{C^2(s)}\Bigg[\left(-2R+\frac{f}{f_R}-\frac{2V}{f_R}+\frac{f_R}{3f_{RR}}+\frac{Rf_Rf_{RRR}}{3f_{RR}^2}+\frac{2\alpha^2}{3}\frac{f_Rf_{RRR}}{A^2f_{RR}^2}\right)\\
&-\left(-2R+\frac{f}{f_R}-\frac{2V}{f_R}+\frac{f_R}{3f_{RR}}+\frac{Rf_Rf_{RRR}}{3f_{RR}^2}+\frac{2\alpha^2}{3}\frac{f_Rf_{RRR}}{A^2f_{RR}^2}\right)\bigg|_{\phi_A}\Bigg].
\end{aligned} \tag{E.17}$$

As is evident from these expressions, and analogous to the case of the FLRW metric with positive curvature, while general expressions may be formulated, performing the explicit calculations presents significant challenges. Consequently, such an analysis lies beyond the scope of the present work.

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