

UNIVERSIDAD COMPLUTENSE DE MADRID
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TESIS DOCTORAL

Dark Energy, Cosmological Singularities and their Quantum Fate:
Insights from Scalar-Tensor Theories and Metric $f(R)$ Gravity

Energía Oscura, Singularidades Cosmológicas y su Destino Cuántico:
Perspectivas desde las Teorías Escalar-Tensor y la Gravedad Métrica $f(R)$

MEMORIA PARA OPTAR AL GRADO DE DOCTOR

PRESENTADA POR

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Facultad de Ciencias Físicas
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Dissertation submitted for the degree of Doctor of Philosophy in Physics by

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Abstract

This PhD dissertation explores scalar-tensor theories and other modifications to general relativity to address fundamental questions about the origin of the late-time acceleration of the Universe and the role of dark energy in shaping its ultimate fate. In particular, our research has focused on scalar-tensor theories known as kinetic gravity braiding and on modification of the Einstein-Hilbert action in the form of metric $f(R)$ theories of gravity, in both of which gravitational waves trivially propagate at the speed of light.

In the context of scalar theories, special attention is placed on the shift-symmetric version of the kinetic gravity braiding theory. We impose a shift symmetry in these scalar theories since this symmetry potentially leads to the avoidance of some fine-tuning problems. These scalar theories are well-known not only for the possibility of driving the expansion of the cosmos towards a future self-tuning de Sitter state, but also for allowing a stable phantom crossing. Hence, they offer an interesting theoretical foundation for exploring dark energy dynamics. Using a dynamical systems approach, we investigate the general future evolution of shift-symmetric kinetic gravity braiding models. Our analysis reveals that the self-tuning de Sitter states traditionally associated with this shift-symmetric scalar theories may not always be the only attractor solutions; instead, a variety of singular outcomes, like big rip scenarios, can emerge.

Analysing the stability of scalar linear perturbations, we also discuss the conditions that seem to be necessary to describe (super) accelerated cosmic expansion without introducing instabilities in the cosmological perturbations. However, it has been previously established that the linearised analysis does not guarantee the stability of this non-canonical scalar theory, as potentially dangerous interactions between dark energy fluctuations and tensor perturbations (essentially gravitational waves) appear at higher order in perturbation theory. Indeed, although we shall point out that the standard proof of absence of dark energy stable braiding models due to this interaction has a possible way-out, we find general arguments suggesting that there are no dark energy stable solutions that can exploit this loophole. Thus, we discuss future research directions for finding viable fundamental descriptions of dark energy that can avoid this detrimental interaction.

In the second part of this PhD dissertation, we explore the equivalence between the background classical cosmic evolution associated with a given dark energy model in general relativity and its counterpart within the framework of metric

Abstract

$f(R)$ theories of gravity, where the accelerated expansion arises from a purely geometrical origin. Focusing on specific phantom dark energy models that have been constrained by observational data, we investigate the emergence of future cosmological singularities—namely, the big rip, little rip, and the little sibling of the big rip—within the context of metric $f(R)$ theories of gravity. These singularities describe extreme cosmological scenarios in which all bound structures and, ultimately, the very fabric of spacetime itself are destroyed.

However, as these classical singularities are approached, quantum effects may become significant. To address this regime, we explore the quantum cosmology framework given by the Wheeler-DeWitt equation being adapted for the case of $f(R)$ gravity. Within this context, we apply the DeWitt criterion, demonstrating the existence of solutions to the Wheeler-DeWitt equation in which the wave function vanishes when approaching the regions of the minisuperspace corresponding to the aforementioned cosmological events. This outcome suggests that, as it happens when the gravitational interaction is that provided by general relativity, these classically catastrophic singularities may be avoided due to quantum gravitational effects. Consequently, our findings hint at the potential resolution of these cosmological doomsdays within the framework of metric $f(R)$ theories of gravity.

Resumen

Esta disertación doctoral explora diversas teorías escalar-tensor y otras modificaciones a la relatividad general para abordar preguntas fundamentales sobre el origen de la aceleración tardía del Universo y el papel de la energía oscura en definir su destino final. En particular, nuestras investigaciones se han centrado en teorías escalar-tensor conocidas como *kinetic gravity braiding* y en la modificación de la acción de Einstein-Hilbert mediante teorías métricas de gravedad $f(R)$, donde en ambas teorías las ondas gravitacionales se propagan de forma natural a la velocidad de la luz.

En el contexto de las teorías escalares, se presta especial atención a la versión con simetría de desplazamiento de la teoría conocida como *kinetic gravity braiding*. Imponemos esta simetría en estas teorías escalares ya que podría ayudar a evitar algunos problemas de ajuste fino. Estas teorías son ampliamente conocidas no solo por la posibilidad de impulsar la expansión del cosmos hacia un estado futuro de autoajuste de tipo de Sitter, sino también por permitir un cruce fantasma estable. Por lo tanto, ofrecen una base teórica interesante para explorar la dinámica de la energía oscura. Mediante un enfoque de sistemas dinámicos, investigamos la evolución futura general de los modelos de *kinetic gravity braiding* con simetría de desplazamiento. El análisis revela que los estados de tipo de Sitter de autoajuste tradicionalmente asociados con estas teorías escalares con simetría de desplazamiento no siempre son soluciones atractoras; en su lugar, pueden surgir diversos resultados singulares, como escenarios de gran desgarramiento (big rip).

Analizando la estabilidad de las perturbaciones escalares lineales, también discutimos las condiciones que parecen ser necesarias para describir una expansión cósmica (súper)acelerada sin introducir inestabilidades en las perturbaciones cosmológicas. Sin embargo, se ha establecido previamente que el análisis linealizado no garantiza la estabilidad de esta teoría escalar no canónica, ya que aparecen interacciones potencialmente peligrosas entre las fluctuaciones de la energía oscura y las perturbaciones tensoriales (esencialmente ondas gravitacionales) en órdenes superiores de la teoría de perturbaciones. De hecho, aunque señalamos que la prueba estándar de la ausencia de modelos estables de energía oscura con braiding debido a esta interacción tiene una posible excepción, encontramos argumentos generales que sugieren que no existen soluciones estables de energía oscura que puedan aprovechar esta laguna. Por ello, discutimos posibles direcciones de investigación futura para encontrar descripciones fundamentales viables de la energía

Resumen

oscura que puedan evitar esta interacción perjudicial.

En la segunda parte de esta disertación doctoral, exploramos la equivalencia entre la evolución clásica cosmológica de fondo asociada a un modelo determinado de energía oscura en el marco de la relatividad general y su contraparte dentro de las teorías métricas de gravedad $f(R)$, donde, en este último enfoque, la expansión acelerada del universo surge de un origen puramente geométrico. Centrándonos en modelos específicos de energía oscura tipo fantasma que han sido restringidos por datos observacionales, investigamos la aparición de singularidades cosmológicas futuras —a saber, el *big rip*, el *little rip* y el *little sibling of the big rip*— dentro del contexto de las teorías métricas $f(R)$ de gravedad. Estas singularidades describen escenarios extremos en los cuales todas las estructuras ligadas del universo y, en última instancia, el propio tejido del espacio-tiempo se destruyen.

No obstante, a medida que la evolución del universo se aproxima a estas singularidades clásicas, los efectos cuánticos pueden volverse significativos. Para abordar este régimen, exploramos el marco de la cosmología cuántica dado por la ecuación de Wheeler-DeWitt adaptada al caso de la gravedad métrica $f(R)$. En este contexto, aplicamos el criterio de DeWitt, demostrando la existencia de soluciones a la ecuación de Wheeler-DeWitt en las cuales la función de onda se anula al aproximarse a las regiones del minisuperespacio correspondientes a los eventos cosmológicos mencionados. Este resultado sugiere que, al igual que ocurre cuando la interacción gravitatoria está descrita por las leyes de la relatividad general, estas singularidades cosmológicas podrían ser evitadas debido a los efectos de la gravedad cuántica. En consecuencia, nuestros hallazgos apuntan a una posible resolución de estos escenarios catastróficos dentro del marco de las teorías métricas de gravedad $f(R)$.

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Notations and conventions

Greek letters denote the four-dimensional spacetime indices 0123. Latin letters are used for the three-dimensional spatial indices 123.

We employed the mostly plus metric signature $(-, +, +, +)$.

The geometric unit system $8\pi G = c = 1$ is used throughout the thesis.

Riemann tensor $R_{\nu\rho\sigma}^{\mu} = \partial_{\rho}\Gamma_{\nu\sigma}^{\mu} - \partial_{\sigma}\Gamma_{\nu\rho}^{\mu} + \Gamma_{\rho\lambda}^{\mu}\Gamma_{\nu\sigma}^{\lambda} - \Gamma_{\sigma\lambda}^{\mu}\Gamma_{\nu\rho}^{\lambda}$.

Ricci tensor $R_{\nu\sigma} = R_{\nu\mu\sigma}^{\mu}$.

Scalar curvature $R = g^{\nu\sigma}R_{\nu\sigma}$.

The symmetrization and anti-symmetrization of indices run as follows

$$A_{(\mu\nu)} = \frac{1}{2}(A_{\mu\nu} + A_{\nu\mu}) \quad \text{and} \quad A_{[\mu\nu]} = \frac{1}{2}(A_{\mu\nu} - A_{\nu\mu}).$$

The kinetic term for the scalar field ϕ is defined as $X := -\frac{1}{2}g^{\mu\nu}\nabla_{\mu}\phi\nabla_{\nu}\phi$.

The covariant d'Alembertian operator is defined as $\square := g^{\mu\nu}\nabla_{\mu}\nabla_{\nu}$.

Given a function $f(x, y, \dots)$, we often use the shorthand notation f_x to express partial derivatives, i.e. $f_x = \frac{\partial f}{\partial x}$.

List of abbreviations

Λ CDM	Λ -Cold-Dark-Matter	6
BB	Big Bang	46
BF	Big Freeze	47
BO	Born-Oppenheimer (approximation)	142
BR	Big Rip	46
CMB	Cosmic Microwave Background	15
CPL	Chevallier-Polarski-Linder (parametrization)	19
DE	dark energy	6
DEC	Dominant Energy Condition	9

Notations and conventions

DESI	Dark Energy Spectroscopic Instrument	19
DHOST	Degenerated Higher-Order Scalar-Tensor (theory)	22
DM	dark matter	6
DOF	degree of freedom	20
dS	de Sitter (state)	26
DW	DeWitt (criterion)	53
EDE	Early Dark Energy	106
EFT	Effective Field Theory	17
EOS	equation of state	17
FLRW	Friedmann-Lemaître-Robertson-Walker (metric)	6
GLPV	Gleyzes-Langlois-Piazza-Vernizzi (theory)	22
GR	General Relativity	5
GWs	gravitational waves	20
KGB	Kinetic Gravity Braiding	21
LR	Little Rip	49
LSBR	Little Sibling of the Big Rip	49
mWDW	modified Wheeler-DeWitt (equation)	120
NCC	Null Convergence Condition	10
NEC	Null Energy Condition	10
SEC	Strong Energy Condition	10
TCC	Time-like Convergence Condition	10
w.r.t.	with respect to	8
WDW	Wheeler-DeWitt (equation)	52
WEC	Weak Energy Condition	9

Publications

Peer-reviewed publications during the PhD programme:

- [1] T. Borislavov Vasilev, M. Bouhmadi-López and P. Martín-Moruno, “Dark energy with a shift-symmetric scalar field: obstacles, loophole hunting and dead ends,” *Phys. Dark Univ.* **46** (2024) 101679, arXiv:2406.12576 [gr-qc].
- [2] T. Borislavov Vasilev, M. Bouhmadi-López and P. Martín-Moruno, “Phantom attractors in kinetic gravity braiding theories: a dynamical system approach,” *JCAP* **06** (2023), 026, arXiv:2212.02547 [gr-qc].
- [3] T. Borislavov Vasilev, M. Bouhmadi-López and P. Martín-Moruno, “Big rip in shift-symmetric Kinetic Gravity Braiding theories,” *Phys. Lett. B* **838** (2023), 137711, arXiv:2210.07276 [gr-qc].
- [4] T. Borislavov Vasilev, M. Bouhmadi-López and P. Martín-Moruno, “Classical and Quantum $f(R)$ Cosmology: The Big Rip, the Little Rip and the Little Sibling of the Big Rip,” *Universe* **7** (2021) no.8, 288, arXiv:2106.12050 [gr-qc].
- [5] T. Borislavov Vasilev, M. Bouhmadi-López and P. Martín-Moruno, “Little rip in classical and quantum $f(R)$ cosmology,” *Phys. Rev. D* **103** (2021) no.12, 124049, arXiv: 2103.12786 [gr-qc].

Other publications related to the content of this thesis:

- [6] T. Borislavov Vasilev, M. Bouhmadi-López and P. Martín-Moruno, “Classical and quantum fate of the little sibling of the big rip in $f(R)$ cosmology,” *Phys. Rev. D* **100** (2019) no.8, 084016, arXiv:1907.13081 [gr-qc].

Part I

Introduction

1

The standard cosmological paradigm

THE DEPTHS of the firmament have aroused the curiosity and wonder of humanity since the dawn of time. Questions about the nature, origin and fate of the Universe have always been present in people’s minds, the answers to which have historically been intertwined in non-trivial ways not only with the philosophical and scientific viewpoints at the time, but also with the theological and mythological beliefs of the society. As a result, the cosmological perception of humanity throughout history has been strongly idiosyncratic: being a byproduct of and, at the same time, actively shaping the traditions and culture of humankind. It is only in recent times (within the last century) that Cosmology has matured into a full-fledged scientific research field, fundamentally transforming our understanding of the cosmos.

The dominant perception about the structure of the Universe throughout recent history has been undoubtedly influenced by the Celestial Orbs model (see figure 1.1a) as presented by Claudio Ptolemy in his famous treatise on the apparent motions of the stars and planetary orbits: the *ALMAGEST*¹. Written in the 2nd-century, its impact extended from Hellenistic Alexandria to the medieval Byzantine and Islamic realms, and persisted across Western Europe during the Middle Ages and early Renaissance. The known Universe (Solar System + brightest stars) is structured in concentric spherical shells with the Earth at the very centre. Each shell contains and aims to explain the apparent motion of some of the objects in the skies as perceived at the time. However, this hierarchical and geocentric view of the Universe was not only used to understand the apparent motion of the skies, but also to address questions related to the existence of vacuum, the composition of outer space, the size of the cosmos, etc. Subjected to minor adjustments over time, this framework persisted as the dominant paradigm until the Newtonian theory provided a unifying synthesis, completing the gradual transition initiated by Copernicus’s revolutionary ideas and advanced by the contributions of Brahe, Galileo, Kepler and others [7].

Grounded on fundamental theories of physics and supported by cutting-edge-technology observations, Modern Cosmology provides humanity with a completely different image of our Universe. Significantly bigger in size and complexity, homogeneity and isotropy play a central role in the modern view of the Universe:

¹The name of the Arabic transcription of the original Greek manuscript.

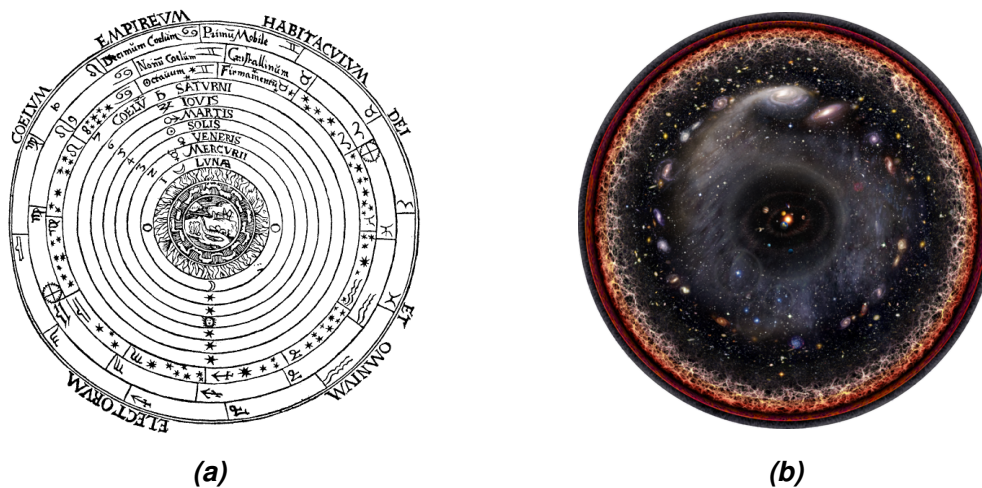


Figure 1.1: (a) Geocentric conception of the Universe as a series of concentric spheres. Credit: P. Apianus, *Cosmographia* (1539); picture from <https://commons.wikimedia.org/wiki/File:Ptolemaicsystem-small.png> under public domain. (b) Artistic composition of the observable universe with the Solar System at the centre. Credit: https://commons.wikimedia.org/wiki/File:Observable_universe_logarithmic_illustration.png by Pablo Carlos Budassi© under license CC BY-SA 3.0.

no preferred position exists within it. The new properties of general relativity, the observation that the Universe is expanding, and the idea that the (classical) Universe is not past-infinite in time, have also introduced the notion of *horizons* in modern cosmology. The Universe may be spatially infinite, but we can only observe a finite patch of it: the observable universe. In a very broad sense, and not without a bit of poetic license, the observable universe becomes observer-centred again, although no preferred observer exists! Each one is at the centre of his own observable patch of this vast Universe (see figure 1.1b), at least as far we consider the predictions of the classical theory to its limits.

1.1 General Relativity and Modern Cosmology: a brief overlook on the cosmological constant

Modern Cosmology (thereon referred to as Cosmology) is the scientific study of the origin, evolution, and structure formation of the Universe. It is the branch of modern science that explores the large scale properties and dynamics of the cosmos, as well as its possible ultimate fate(s). Although cosmology has experi-

enced a massive development during the last century, in both its theoretical and observational aspects, it is a relatively young field of research. It matured as an independent scientific field only after the publication of General Relativity (GR) in 1915 [8]. The theory of GR describes the deformation of spacetime due to the presence of matter-energy through the famous Einstein's field equations

$$R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} = \frac{8\pi G}{c^4}T_{\mu\nu}, \quad (1.1)$$

where $R_{\mu\nu}$ is the Ricci tensor, R the scalar curvature, $g_{\mu\nu}$ stands for the spacetime metric and $T_{\mu\nu}$ is the energy-momentum tensor describing the spacetime distribution of matter. In the following, we will adopt the geometric unit system in which $8\pi G = c = 1$.

Two years after the publication of GR, Einstein himself applied the new theory of relativity to the Universe as a whole [9]. However, it is important to note that by 1917 the known Universe did not effectively exceed the Milky Way (see for instance reference [10]). The idea that some nebulae actually represent distant *island universes* or *galaxies* can be traced back to the 18th century, with Thomas Wright, Immanuel Kant, and William Herschel as key contributors [11]. The idea of extragalactic objects gained momentum in the 19th century, supported by observations of the complex spiral-like structures of some nebulae, such as those recorded by William Parsons in 1845 [12]. In the early 20th century, additional evidence emerged with the detection of several Novae in spiral nebulae (see 1917's publication [13]) and the onset of nebular spectroscopy, which led to the first detection of blue/redshift in spiral nebulae by Vesto Slipher [14]. However, it was not until the Shapley-Curtis Debate (The Great Debate) in 1920 that the extragalactic nature of spiral nebulae began to gain consensus, expanding the perceived size and complexity of the universe (see [11] for an historical analysis). Definitive proof arrived in 1925 when Edwin Hubble resolved individual Cepheid variables within the Andromeda galaxy [15], and a few years later, in 1929, he established the linear relationship between redshift and distance—now known as Hubble's law [16]. Thus, strong evidence for a vast, non-static universe only fully emerged with Hubble's work in 1929. It is in this historical context that Einstein, in 1917, slightly modified his theory in order to accommodate static solutions describing a spatially finite universe. The modification run as follows

$$R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} + \Lambda g_{\mu\nu} = T_{\mu\nu}, \quad (1.2)$$

where Λ is a *universal constant* introduced *ad hoc* to counteract the gravitational collapse of uniformly distributed matter [9]. A constant he will soon heavily regret having introduced, but will be re-embraced as the Cosmological Constant of the standard cosmological model at the end of the century.

During this cosmo-awakening period, Alexandre Friedmann (1922) showed that the modified Einstein field equations (1.2) also admit non-static solution describing an evolving universe [17]. Unaware of Friedmann's work, George Lemaître deduced in 1927 the same non-static solution [18]. Remarkably, the motivation of Lemaître's pioneering work was to explain the observed recession velocity of spiral nebulae as a consequence of the expansion of the Universe. He also discussed for the first time the thermodynamics of an expanding universe, introduced matter and radiation energy densities in the cosmological setting, and (in a subsequent paper [19]) proposed a proto-Big-Bang picture. Later, Howard Robertson in 1929 [20] and Arthur Walker in 1935 [21] independently proved that the Friedmann-Lemaître solution was indeed the most general model for the universe consistent with homogeneity and isotropy. Nowadays, we know this non-static solution as the Friedmann-Lemaître-Robertson-Walker (FLRW) metric.

By 1931 Einstein was already public on rejecting the idea of his fine-tuned universal constant [10]. The reason for this change of mind is basically twofold. On theoretical grounds, he was aware that the static model was unstable. Small perturbations around the static arrangement brings the model either into expansion or collapse. On empirical grounds, there was no more need of the term since the assumption of stasis was no longer observationally justified. After that, the universal constant was largely ignored by physicists for several decades.

The discovery in the late 90's signalling that our universe is not only expanding but currently undergoing an accelerated expansion phase, supposed another inflexion point in our conception of the physics of the cosmos. Even though this acceleration was first noticed more than twenty years ago [22, 23], its mysteries are still today not fully unravelled. On the contrary, understanding the mechanism involved in this phase represents one of the greatest milestones in modern cosmology. This behaviour is so challenging because no form of matter we know from our ordinary experience can actually produce this phenomenon. In GR, this phase is attributed to the existence of an exotic form of energy with sufficiently negative pressure that causes the repulsion of the matter content and, thus, pushes the universe further into expansion. This exotic content is dubbed dark energy (DE) and the description of this dark content is the central topic of this thesis. The historical approach, also the simplest and still the one with the overall best fit to the observational data, is that of the standard Λ -Cold-Dark-Matter (Λ CDM) model where Einstein's universal constant (now renamed as the cosmological constant) plays the role of DE. Nevertheless, this model contains various theoretical and observational unresolved puzzles which have often served as motivation for exploring alternative description for this phenomenon. To mention some of them: the nature of dark matter (DM) and DE [24–29], the coincidence problem [30], the cosmological constant problem [31] and the new tensions arising in certain

cosmological parameters [32, 33]. Updated reviews on the topic may be found in, for instances, references [34, 35] and references therein.

1.2 Energy-momentum tensor

The famous quote by J. Wheeler² “Space tells matter how to move. Matter tells space how to curve” resumes perfectly the spirit of the geometric approach for describing the gravitational interaction. The theory of GR, or any other metric theory of gravity, spells how the geometry of spacetime is affected by the mass-energy distribution within it, and how this distribution changes due to the evolution of the spacetime. The relevant information about the *matter* content of the classical theory is captured in the covariantly conserved energy-momentum tensor $T_{\mu\nu}$. Hence, in this section we review the different ways of characterising this tensor: the fluid description and the action description.

1.2.1 Fluid description

Let n^μ be a unit time-like four-vector, i.e. $n_\mu n^\mu = -1$, representing the four-velocity of a fluid. Then, the energy-momentum tensor associated to that fluid can be expressed in the form [38, 39]

$$T_{\mu\nu} = (\varrho + p)n_\mu n_\nu + pg_{\mu\nu} - 2q_{(\mu}n_{\nu)} + \pi_{\mu\nu}, \quad (1.3)$$

where $q_\mu n^\mu = 0$, $\pi_\mu^\mu = 0$, $\pi_{\mu\nu} = \pi_{(\mu\nu)}$ and $u^\mu \pi_{\mu\nu} = 0$. In this decomposition, ϱ and p represent the total energy density and isotropic pressure measured at any time by an observer co-moving with n^μ . That is, the energy density and isotropic pressure of the fluid as measured in its rest-frame. Similarly, q^μ represents the energy flux relative to the time-like direction n^μ , and $\pi_{\mu\nu}$ stands for the anisotropic stress.

In cosmology, the energy-momentum tensor is usually the sum of the different matter forms that populate the universe (e.g. radiation, baryonic matter, etc.). In particular, the *perfect fluid* picture is often invoked to portray (at least) radiation and dust-like matter after recombination. A perfect fluid is described by an energy-momentum tensor that reads [38, 39]

$$T_{\mu\nu}^{\text{p.f.}} = (\varrho + p)n_\mu n_\nu + pg_{\mu\nu}, \quad (1.4)$$

which corresponds to set q_μ and $\pi_{\mu\nu}$ to zero in expression (1.3). However, deviations from the perfect fluid picture can also be important for modelling, for example, DE phenomenology with stability properties different from those of a perfect fluid. This is indeed the case of the scalar field theories known as *kinetic gravity braiding* [40, 41], which represent the central discussion in this thesis.

²Quote from reference [36] p. 7. Further commented by J. Wheeler in [37] p. 234.

1.2.2 Principle of least action

Einstein's field equations can also be obtained from a variational principle. Assuming for simplicity Λ trivial, the left-hand side of equations (1.1) follows from Einstein-Hilbert action [42, 43],

$$S_{\text{EH}}[g^{\mu\nu}] = \frac{1}{2} \int \sqrt{-g} d^4x R, \quad (1.5)$$

being g the determinant of the metric and R the Ricci scalar. Varying this action with respect to (w.r.t.) the metric $g^{\mu\nu}$ results in

$$\frac{\delta S_{\text{EH}}}{\delta g^{\mu\nu}} = \frac{\sqrt{-g}}{2} \left(R_{\mu\nu} - \frac{1}{2} g_{\mu\nu} R \right), \quad (1.6)$$

where we recall that the geometric unit system ($8\pi G = c = 1$) has been adopted.

If the matter content is described by a Lagrangian density $\mathcal{L}_{\text{matter}}$, which depends on the matter fields and their coupling to gravity, the total action reads

$$S = S_{\text{EH}} + S_{\text{matter}}. \quad (1.7)$$

The principle of least action, then, demands

$$\frac{\delta S}{\delta g^{\mu\nu}} = \frac{\delta S_{\text{EH}}}{\delta g^{\mu\nu}} + \frac{\delta S_{\text{matter}}}{\delta g^{\mu\nu}} = 0, \quad (1.8)$$

for the functional dependence on the metric $g^{\mu\nu}$. This results in

$$R_{\mu\nu} - \frac{1}{2} g_{\mu\nu} R = -\frac{2}{\sqrt{-g}} \frac{\delta(\sqrt{-g} \mathcal{L}_{\text{matter}})}{\delta g^{\mu\nu}}. \quad (1.9)$$

Therefore, comparing the above expression with equations (1.1) it is possible to identify the energy-momentum tensor related to $\mathcal{L}_{\text{matter}}$ as

$$T_{\mu\nu} := -\frac{2}{\sqrt{-g}} \frac{\delta(\sqrt{-g} \mathcal{L}_{\text{matter}})}{\delta g^{\mu\nu}}. \quad (1.10)$$

This representation of the energy-momentum tensor will be important in the next chapters when considering scalar field theories as a fundamental framework for addressing the accelerated expansion of the universe.

1.3 Energy conditions

The framework of GR does not provide by itself any specific hint on what kind of matter content is *acceptable*. Indeed, any geometry can satisfy Einstein's field

equations provided the suitable energy-momentum tensor. The (extra) assumptions that can be adopted for the energy-momentum tensor to closely reproduce a *physically reasonable* matter content are the so-called Energy Conditions. These are phenomenological conditions based on our ordinary experience on how *normal matter* should behave independently of the theory of gravity. The energy conditions most often discussed in modern literature are the *weak, dominant, strong* and *null* energy conditions [44–48].

Weak Energy Condition (WEC) This condition ensures that the energy density measured by any observer is non-negative, which demands [44, 45, 47]

$$T_{\mu\nu}n^\mu n^\nu \geq 0, \quad (1.11)$$

for any time-like vector n^μ . Particularised to the case of a perfect fluid, this implies that [47, 48]

$$\varrho \geq 0 \quad \text{and} \quad \varrho + p \geq 0, \quad (1.12)$$

for an energy-momentum tensor in the form of expression (1.4).

Dominant Energy Condition (DEC) The energy density measured by any observer is non-negative and propagates locally in a causal way. This implies [44, 45, 47]

$$T_{\mu\nu}n^\mu n^\nu \geq 0 \quad \text{and} \quad (-T_\alpha^\mu n^\alpha)(-T_{\mu\beta}n^\beta) \leq 0, \quad (1.13)$$

for any time-like vector n^μ . This condition is fulfilled when [47, 48]

$$\varrho \geq |p| \geq 0, \quad (1.14)$$

for a perfect fluid (1.4).

It is important to highlight, however, that if we are interested in analysing general properties of the spacetime without invoking a detailed characterization of the matter fields, then, purely geometrical statements (or relations) should be considered; for instance, the Raychaudhuri equation describing the focusing of a congruence of time-like (or null) curves. Particularized to geodesic motion, this reads [38, 44]

$$\frac{d\theta}{d\tau} = \omega_{\mu\nu}\omega^{\mu\nu} - \sigma_{\mu\nu}\sigma^{\mu\nu} - \frac{1}{3}\theta^2 - R_{\mu\nu}n^\mu n^\nu, \quad (1.15)$$

where τ is the affine parameter along the geodesic, n^μ is a time-like unit vector tangent to the congruence, $\omega_{\mu\nu}$ is the vorticity of the congruence, $\sigma_{\mu\nu}$ represents

the shear and θ measures the expansion. For vorticity-free congruences, in which case the tangent vector can be expressed as a gradient of a scalar field [49], the only possible term that may not have a negative sign in the above expression is the last one. Therefore, if $R_{\mu\nu} n^\mu n^\nu \geq 0$ for any time-like vector n^μ , then, geodesics converge, since the expansion scalar θ decreases always. The converse is not, however, automatically true: $R_{\mu\nu} n^\mu n^\nu < 0$ does not imply that the right-hand side of expression (1.15) is positive and, therefore, defocusing of geodesics [50]. The condition $R_{\mu\nu} n^\mu n^\nu \geq 0$ for any time-like vector n^μ is known as the Time-like Convergence Condition (TCC), and it guarantees that gravity is always an attractive force. Please note that this is a general (geometrical) statements that do not assume any particular theory of gravity, but relies only on the validity of geodesic motion for free-falling observers. The same line of reasoning can also be extended to null geodesics [38, 44]. Considering a null congruence with tangent vector v^μ , the condition $R_{\mu\nu} v^\mu v^\nu \geq 0$ for any light-like vector v^μ ensures focusing of null geodesics. Parallel to the previous scenario, this condition is known as the Null Convergence Condition (NCC). Let us recall again that the TCC and NCC are purely geometrical statements. Indeed, they are key ingredients in geodesic incompleteness theorems [44, 50]. Moreover, since $R_{\mu\nu}$ depends on the stress–energy tensor through the equations of the dynamics, these conditions also impose restrictions on the material content once the theory of gravity is specified. For example, the TCC leads to the so-called *strong energy condition* in GR.

Strong Energy Condition (SEC) This conditions states that [44, 45, 47]

$$\left(T_{\mu\nu} - \frac{1}{2} T g_{\mu\nu} \right) n^\mu n^\nu \geq 0, \quad (1.16)$$

for any time-like vector n^μ . Using the background equations (1.1) of GR, this condition directly translates to $R_{\mu\nu} n^\mu n^\nu \geq 0$, which is just the TCC. Therefore, the SEC guarantees that gravity is always attractive in GR. This condition can be re-expressed as [47, 48]

$$\varrho + p \geq 0 \quad \text{and} \quad \varrho + 3p \geq 0, \quad (1.17)$$

for an energy-momentum tensor in the form of a perfect fluid (1.4).

Null Energy Condition (NEC) This condition is equivalent to demand that SEC and WEC are satisfied in the limit of null observers [44, 45, 47]. That is

$$T_{\mu\nu} v^\mu v^\nu \geq 0, \quad (1.18)$$

for any light-like vector v^μ . In GR, this is completely equivalent to the NCC [47]. The NEC can be also expressed as [47, 48]

$$\varrho + p \geq 0, \quad (1.19)$$

for an energy-momentum tensor in the form of a perfect fluid (1.4).

Other energy conditions not so popular in modern literature, or believed to be true in the past but completely ruled out nowadays, can be found in [46, 51, 52] and references therein. Manifestly non-linear energy conditions have been discussed in [47]. Contrary to the classical point-wise energy conditions introduced above, conditions on *average* along causal (time-like and null) geodesics and semi-classical conditions have also been debated [47, 48]. Although the energy conditions offer a practical way to enforce the empirical ideas that momentum-energy is *positive* in the presence of matter and that gravity is always an attractive force, they may not actually be related to fundamental physics [47] (see also, for instance, references [53, 54] for the opposite point of view). Indeed, vast evidence indicates that the SEC should be violated in GR to produce the observed late-time accelerated expansion of the universe [22, 23], as well as during the early inflationary epoch [55–57] (see also the review in [58]). Moreover, violations of the NEC have also been discussed in several scenarios [48, 59–65], where an interesting theoretical and experimental example is that of the Casimir effect [66] (see also references [67, 68]). It should be noted that the violation of the NEC automatically imply (by construction) the violation of the other conditions as well. It is well-known, however, that violations of the NEC may signal the presence of instabilities and/or other pathological behaviours [69–71], although stable violations of the NEC are also possible [40, 72, 73]. We will return to this discussion in more details in chapter 5. Finally, it should be also kept in mind that the connection between the TCC (or NCC) and the SEC (or NEC) is valid within GR. Moreover, this connection arises from imposing the latter to the whole energy-momentum tensor, not just to some of the species that independently contributed to it. We will repeatedly insist on this difference when discussing the violation of the NEC in chapter 5. Finally, note that the relation between the convergence conditions and the energy conditions is altered in modified theories of gravity [74, 75].

1.4 The standard cosmological model

The standard cosmological model is based on the *Cosmological Principle*. That is the assumption that the Universe is homogeneous and isotropic when observed on a large enough scale. As a consequence, observations about the structure of the Universe should be independent of the location of the observer and the direction of the measurements.

1.4.1 The Friedmann-Lemaître-Robertson-Walker universe

Homogeneity and isotropy are realised by the FLRW solution to the field equations of GR. In spherical coordinates, this metric is given by the line element [38]

$$ds^2 = -dt^2 + a(t)^2 \left(\frac{dr^2}{1 - kr^2} + r^2 d\theta^2 + r^2 \sin^2 \theta d\varphi^2 \right), \quad (1.20)$$

where t stands for the cosmic time, a represents the scale factor, and k provides the three-dimensional spatial curvature: -1 for open Euclidean sections, 0 for flat profile, and $+1$ for spatially closed geometry. In this manuscript, we will mainly consider the flat scenario. Therefore, we shall focus on the simpler line element [38]

$$ds^2 = -dt^2 + a(t)^2 d\Omega_3^2, \quad (1.21)$$

being $d\Omega_3^2$ the spatially flat euclidean sections. Accordingly, the scalar curvature for the spatially flat FLRW reads [38]

$$R = 6 \left(\dot{H} + 2H^2 \right), \quad (1.22)$$

being $H := \dot{a}/a$ the Hubble rate for the expansion of the universe and where the dot represents derivation w.r.t. the cosmic time t .

The standard cosmological model describes a FLRW universe filled with four different species: *i*) ultra-relativistic matter in the form of photons and light neutrinos, *ii*) pressureless non-relativistic baryonic matter, *iii*) non-relativistic and weakly-interacting *cold* DM, and *iv*) the cosmological constant. In the late universe, the four species are effectively described with a perfect fluid approach, that is, they are characterised by an energy density and a (isotropic) pressure. For the flat FLRW metric, the Einstein's field equations (1.2) reduce to the Friedmann and Raychaudhuri equations

$$3H^2 = \varrho_r + \varrho_m + \Lambda, \quad (1.23)$$

$$\dot{H} = -\frac{1}{2} \left(\varrho_m + \frac{4}{3}\varrho_r \right), \quad (1.24)$$

respectively, where ϱ_r is the energy density for ultra-relativistic matter (hereon referred to as radiation), $\varrho_m = \varrho_b + \varrho_{DM}$ is the energy density for the non-relativistic matter content of the universe (hereon referred to as dust matter or, simply, matter), and Λ represents the cosmological constant, which acts as a DE source driving the current accelerated expansion of the universe. In addition to the above field

equations, the evolution of matter and radiation densities follows directly from the covariant conservation of the corresponding energy-momentum tensor. These are

$$\dot{\varrho}_m + 3H\varrho_m = 0, \quad (1.25)$$

$$\dot{\varrho}_r + 4H\varrho_r = 0. \quad (1.26)$$

Equations (1.23) to (1.26) completely determine the background evolution of the standard model. However, it is important to note that the system (1.23)-(1.26) is overdetermined. This is because there are three dynamical equations and one constraint. Hence, as will be emphasised in the following, the Friedmann constraint equation (1.23) can be used to eliminate either (1.24), (1.25) or (1.26) from the set of *truly* independent equations that fully characterises the dynamics.

The expansion history of the standard model follows by noting that equations (1.25) and (1.26) can be trivially integrated to give

$$\varrho_m(a) = \varrho_m^{(0)} \left(\frac{a}{a_0} \right)^{-3}, \quad (1.27)$$

$$\varrho_r(a) = \varrho_r^{(0)} \left(\frac{a}{a_0} \right)^{-4}, \quad (1.28)$$

where a_0 , $\varrho_m^{(0)}$ and $\varrho_r^{(0)}$ are integration constants derived from the initial conditions. Thus, the Friedmann equation (1.23) can be re-expressed as³

$$3H^2 = \varrho_r^{(0)} \left(\frac{a}{a_0} \right)^{-4} + \varrho_m^{(0)} \left(\frac{a}{a_0} \right)^{-3} + \Lambda, \quad (1.29)$$

which signals the presence of three different stages. The (classical) universe starts in a radiation-dominated epoch at small scale factors. As radiation and matter dilutes with the expansion, the DE component (in the form of the cosmological constant) inevitably dominates the dynamics of the universe. Depending on the initial conditions, an intermediate matter-dominated stage where $H^2 \approx a^{-3}$ may also occur, which is necessary for structures to form.

The Λ CDM model provides an excellent fit to a large span of cosmological data. In this sense, it is overall the most *complete* cosmological model currently available in the market. Nevertheless, this model contains various theoretical and observational unresolved puzzles, which often have served as motivations for studying models beyond Λ CDM. To mention some of them: the nature of DM

³This is the standard model of the hot big-bang cosmology, which has two well-known shortcomings: the horizon and flatness problems [76]. These challenges are addressed by incorporating an inflationary phase preceding radiation dominance [76]. However, we will not take into consideration this early inflationary stage, as our primary focus lies on late-time cosmology.

and DE [24–29], the coincidence problem [30], the cosmological constant problem [31, 77] and the new statistical tensions arising in certain cosmological parameters [32, 33]. In the following we will briefly introduce the latter two issues. Further information about this topic may be found in, for instances, references [34, 35] and references therein.

1.4.2 The cosmological constant problem

Dark energy is the dominant component today [78, 79]. Moreover, at least for the most common models that we have, it will be even more dominant in the future as radiation and matter dilutes with the expansion in the standard model. However, modelling this dark component with a cosmological constant leads a profound theoretical and observational problem (see, for instance, references [24, 25]).

In a nutshell, the problem boils down to the fact that vacuum energy gravitates in GR. In particular, this applies to the zero-point energy of quantum matter fields if we consider semi-classical correction to GR in the form of expectation values of the energy momentum tensor. Moreover, this zero-point vacuum energy contributes to the total energy budget just like a cosmological constant. As a result, an effective cosmological constant emerges in the form of

$$\Lambda_{\text{eff}} = \Lambda + \langle \varrho_{\text{vac}} \rangle, \quad (1.30)$$

where Λ is the *original* cosmological constant appearing in the Einstein-Hilbert action and $\langle \varrho_{\text{vac}} \rangle$ is the sum of the zero-point energies of the quantum matter fields. This effective cosmological constant is indeed the one that enters in the background equation (1.23). Hence, it is observationally constrained to a very small value [79]

$$\Lambda_{\text{eff}} \lesssim H_0^2 \approx 10^{-52} \text{ m}^{-2}. \quad (1.31)$$

On the contrary, the vacuum energy $\langle \varrho_{\text{vac}} \rangle$ is expected to be very large. Therefore, a cancellation between Λ and the vacuum energy must take place. Indeed, the common lore assumes that this cancellation should occur with extraordinary precision over one hundred twenty decimal points [24, 25]. However, this statement follows directly from imposing a cut-off on the quartic ultraviolet divergence of $\langle \varrho_{\text{vac}} \rangle$ at the Planck scale. Nevertheless, it has been shown that this quartic divergence does not actually behave as a cosmological constant, requiring a more refined regularisation [80, 81] (see also [77]).

In any case, it seems that the cancellation between Λ and the vacuum energy would lead to an extreme fine-tuning problem for the value of the cosmological constant. Even worse, the fine-tuned cancellation must also remain robust against radiative corrections to the vacuum energy [77].

1.4.3 Tensions in the standard model

The quality and amount of observational data has significantly increased over the past years. This improvement in the precision of cosmological data has, nevertheless, led to the rise of various statistical tensions between the values of some of the cosmological parameters measured in different experiments. These discrepancies greatly challenge the standard cosmological model and have often served as the main motivation for studying theories beyond Λ CDM. We refer the interested reader to the reviews [32, 33, 35] for a self-contained discussion about the observational tensions in the standard cosmological model.

One of the most stringent discrepancies is the H_0 tension. This is the disagreement between direct and indirect measurements on the current value of the Hubble rate [32]. The latter consists on high redshift probes that extrapolate the late-time H_0 value assuming the Λ CDM model. Typically, these rely on Cosmic Microwave Background (CMB) experiments combined with other lower-redshift observations. Direct surveys, on the other hand, aim to employ Λ CDM-independent local measurements only based on the calibrated distance ladder. Although there are different experiments in each group, the H_0 tension is predominantly driven by the Planck collaboration [79] inferred (i.e. indirect) value of $H_0 = (67.27 \pm 0.60)$ km s⁻¹ Mpc⁻¹ at 68% confidence level, and the SH0ES collaboration [82] direct value of $H_0 = (73.04 \pm 1.04)$ km s⁻¹ Mpc⁻¹ based on the Cepheids-Supernovae at 68% confidence level. These observations alone result in more than 5σ tension. Moreover, the high precision and consistency of the data in both experiments poses significant challenges for a possible solution to the tension. See also reference [83] for historical notes on the determination of H_0 .

Another statistical tension within the standard model usually cited is that related to the S_8 (or σ_8) parameter, which quantifies the strength of matter clustering in the universe (see, for instance, reference [33]). The lower redshift surveys [84, 85], such as weak gravitational lensing and galaxy clustering, generally prefer a lower value of S_8 compared to that estimated from the CMB [79, 86, 87]. Both types of surveys, however, are model dependent in the sense that the Λ CDM model is assumed. In any case, the S_8 tension is at much lower statistical significance than the H_0 tension, reaching between 1.7 to 3 standard deviations depending on the datasets; see for instance [33] and references therein.

2

Dynamical dark energy

AS A RESULT from the theoretical and observational tensions in the Λ CDM model, a great number of alternatives for DE describing the current accelerated phase have been proposed. The various DE proposals can be broadly divided into two groups. The first consists of *modified matter* models for which the energy momentum tensor at the right-hand side of Einstein's equations contains the new exotic form of matter fields with a negative pressure. Some examples are phantom DE [59, 88], tachyonic matter [89, 90], Chaplygin gas [91, 92], holographic DE [93] and scalar fields in the form of quintessence [94, 95] and k-essence [96–98], among others. Alternatively, the current cosmological expansion could be described not by the inclusion of new exotic content but with suitable modifications to the underlying theories of gravity. In that sense, *modified theories of gravity* provide an interesting framework for cosmologists. Some examples of this approach are general scalar field theories *à la* Horndeski [99], beyond Horndeski [100, 101], further generalizations of beyond Horndeski [102–104], Gauss-Bonnet gravity [105, 106], $f(R)$ theories of gravity [107] (see also references [108–111]), $f(R, \mathcal{T})$ gravity [112], where \mathcal{T} stands for the trace of the energy momentum tensor, $f(T)$ modified teleparallel gravity [113], with T being the torsion scalar, and modified symmetric teleparallel $f(Q)$ theories of gravity [114], where Q denotes the non-metricity scalar. For a review on the state of the art in DE please see references [115–118] and references therein.

In this chapter we review the different approaches to a dynamical DE component that are relevant for the content of this thesis. We also introduce the analysis techniques and notation later employed in the main body of the document. The first part of this chapter is devoted to the description of a dynamical DE component at the background level. We start by introducing the phenomenological description of DE by means of an equation of state (EOS) in section 2.1. In section 2.2 we discuss scalar field theories as a fundamental description of an effective DE component. We comment on shift-symmetric scalar fields for the dark sector in section 2.3. Dynamical system approach to DE is introduced in section 2.4. The second part of the chapter deals with DE at the perturbative level. Thus, section 2.5 introduces the main stability criteria for linear scalar perturbations. Meanwhile, in section 2.6 we review the Effective Field Theory (EFT) of DE, which represents a useful approach for describing linear and beyond linear order DE fluctuations around a FLRW background.

2.1 Fluid description of dark energy

From a practical perspective, whatever the origin of DE may be, it can be described effectively as a (dark) fluid characterised by an EOS. In this phenomenological approach, the EOS parameter w of the dark fluid plays an important role. That is the ratio between the pressure and energy density of the DE fluid, or the effective pressure and energy density in the case of modified theories of gravity. In the w -line, the behaviour of dynamical DE models can be broadly divided into three categories. The first one corresponds to Quintessence-like models for which $w > -1$. Covariant conservation of the energy momentum tensor results in a decreasing DE-density with the expansion. In the second place we have the (non-dynamical) cosmological constant case given by $w = -1$. The third possibility is that of $w < -1$, which characterises the so-called phantom energy. These are DE models with very exotic properties as we will discuss in section 3.1. Observational constraints on w are, therefore, crucial to unveil possible hints on the true nature of this exotic content. In this fashion, the currently available cosmological data place tight constraints on the present value of the EOS for DE, namely w_0 , limiting it to a very narrow range around -1 ; see, for instance, the values reported in references [78, 79, 119–127]. Remarkably, the possibility of the expansion of the universe being fuelled by phantom-type DE is not observationally excluded. Furthermore, it is even suggested by some data [79, 128] and could help to alleviate the H_0 tension (see, for instance, references [129, 130]). Worthy to notice, it was also recently shown that a phantom transition is a necessary prerequisite in order to solve both H_0 and S_8 tensions simultaneously with late-time modifications to Λ CDM only [131, 132].

Within the spirit of this phenomenological approach to the DE enigma, in chapter 6 we discuss the cosmological consequences of describing DE with the EOS given by

$$p = -\rho - \mathcal{A}\rho^\alpha, \quad (2.1)$$

where \mathcal{A} and α are constants. This EOS was first introduced in references [133, 134] motivated as a power-law expansion around the cosmological constant case (i.e. $p = -\rho$). The expansion history of a universe filled with (2.1) was thoroughly discussed in reference [135], showing a great variety of possible future evolutions for this dark fluid. Indeed, some of the different scenarios have been tested against observations [136, 137]. In the first part of chapter 6, we will review the analysis performed in reference [135] and present some new conclusions on the phenomenology of this exotic EOS.

For a given DE candidate, the resulting expansion history should be tested against observations. This may turn, however, to be a challenging task given the

increasing proliferation of DE models. Alternatively to this route, one may attempt to reconstruct the properties of DE directly from observations in a nearly model-independent way; see reference [138] for a review on this approach. In particular, we shall briefly mention the w_0w_a CDM parametrization before concluding this section. Also known as the Chevallier-Polarski-Linder (CPL) parametrization [139, 140], it has rather recently gained a renewed interest in light of the latest results from the Dark Energy Spectroscopic Instrument (DESI) in support of a dynamical DE over Λ CDM [127]. The CPL is a two-parameter heuristic description of an unknown DE component under the assumption of a *weak* dependence of w on the redshift. In this approach, a dynamical DE component is modelled as a fluid with an evolving EOS parameter

$$w(z) = w_0 + w_a \frac{z}{1+z}, \quad (2.2)$$

being w_0 and w_a the parameters that shall be constrained using observational probes. This parametrization has been shown compatible with different quintessence and phantom-like scalar field models [141–144], although it may not be an optimal parametrization for testing some other DE candidates [145]. More concretely, it cannot accommodate rapidly varying DE models (see also the review [138]). Worthy to note, this parametrization can also be thought of as an effective low-redshift Taylor expansion of an evolving $w(a)$ parameter around $a = 1$.

Using a CPL characterization, the recent release of DESI measurements [127] of Baryon Acoustic Oscillations in combination with CMB and SNIa data shows a preference for dynamical DE over a cosmological constant (which corresponds to $w_0 = -1$ and $w_a = 0$) at more than 2σ . In particular, $w_0 = -0.827 \pm 0.063$ and $w_a = -0.75^{+0.29}_{-0.25}$ for DESI+CMB+PantheonPlus [127]. Although the results are preliminary and not free of controversy [146–149], these claims have been supported by independent studies [150–152]. In any case, future DESI releases may shed more light on this discussion. It is undeniable, however, that these results have had a significant impact on the community and have contributed to the idea that DE is dynamic in nature.

2.2 Fundamental description of dark energy

Complementary to the effective fluid description, scalar field theories could be crucial in providing an underlying theoretical framework for addressing the mysteries of DE. These theories introduce a scalar field that can be used to describe a dynamical DE, in contrast to the cosmological constant case (see, for instance, references [26, 29, 115]). To select the appropriate scalar field theory for cosmology, it is reasonable to demand that the corresponding field equations are of second

order. Otherwise, the new degree of freedom (DOF) may destabilise the dynamics of the theory by means of the Ostrogradski ghost [153]. In this context, a natural framework is that provided by Horndeski theory [99] (see also [154, 155] for a review). The Horndeski theory was originally proposed in 1974 [99], but it went largely unnoticed until it was recently rediscovered in 2011 [156] when constructing general covariant extensions of the galileons (see also reference [157]). In its modern version, the action of Horndeski theory is given by [158]

$$S_{\text{Horn}} = \int d^4x \sum_{i=2}^5 \mathcal{L}_i, \quad (2.3)$$

where \mathcal{L}_i are all the possible Lagrangian densities built from the scalar field and its first and second derivatives that lead to second order field equations for both the metric and the scalar field. These are [158]

$$\mathcal{L}_2 = K(\phi, X), \quad (2.4)$$

$$\mathcal{L}_3 = -G_3(\phi, X)\square\phi, \quad (2.5)$$

$$\mathcal{L}_4 = G_4(\phi, X)R + G_{4X}(\phi, X) \left[(\square\phi)^2 - \phi_{\mu\nu}\phi^{\mu\nu} \right], \quad (2.6)$$

$$\mathcal{L}_5 = G_5(\phi, X)G^{\mu\nu}\phi_{\mu\nu} - \frac{1}{6}G_{5X}(\phi, X) \left[(\square\phi)^3 + 2\phi_\mu^\alpha\phi_\alpha^\nu\phi_\nu^\mu - 3\phi_{\mu\nu}\phi^{\mu\nu}\square\phi \right], \quad (2.7)$$

being K and G_i four arbitrary functions on the scalar field ϕ and its kinetic term

$$X := -\frac{1}{2}g^{\mu\nu}\nabla_\mu\phi\nabla_\nu\phi, \quad (2.8)$$

where please be aware of the different conventions for the definition of this term throughout the literature [159–162]. In addition, the quantity $\phi_{\mu\nu} := \nabla_\mu\nabla_\nu\phi$ stands for the second derivative of the scalar field, the box represents the covariant d'Alembertian operator $\square\phi := g^{\mu\nu}\nabla_\mu\nabla_\nu\phi$, and the subindex “ X ” symbolise derivation w.r.t. the kinetic term, e.g. $G_{4X} = \partial G_4/\partial X$.

The speed of propagation of gravitational waves (GWs) has also recently become an important factor when formulating theories beyond GR. After the detection of the GWs event GW170817 [163] and its electromagnetic counterpart GRB 170817A [164], it has been concluded that the propagation speed of GWs is very close to that of light in the recent universe [165]. In fact, it was shown that [165]

$$-7 \times 10^{-16} < 1 - c_{\text{GW}} < 3 \times 10^{-15}, \quad (2.9)$$

being c_{GW} the speed of the GWs, where we recall that we have adopted the geometric units in which the speed of light is equal to one. It is interesting to note that

similar bounds had been previously obtained in the context of the gravitational analogue of the Cherenkov radiation applied to high energy cosmic rays [166, 167]. It was also argued in reference [166] that the upper limit for the GWs speed defect (w.r.t. to the speed of light) in equation (2.9) can be made orders of magnitude tighter by invoking cosmic rays of extragalactic origin.

For a flat FLRW background metric, the speed of propagation of GWs in the Horndeski theory (2.3) is given by [168]

$$c_{\text{GW}} = \frac{G_4 - X \left(\ddot{\phi} G_{5X} + G_{5\phi} \right)}{G_4 - 2X G_{4X} - X \left(H \dot{\phi} G_{5X} - G_{5\phi} \right)}, \quad (2.10)$$

which depends on the quartic and quintic Horndeski functions. Consequently, matching the observational constraints in equation (2.9) with the theoretical predictions may result in strong constraints on the Horndeski family. As it was argued in the references [169–171], this observational constraint advocates for the identification of the theoretical models that trivially propagate GWs at the speed of light¹. In this context, the demand of $c_{\text{GW}} \equiv 1$ is realised if and only if the conditions [169–171]

$$G_{4X} = 0 \quad \text{and} \quad G_5 = 0, \quad (2.11)$$

hold true. As a result, the original Horndeski theory (2.3) reduces to²

$$S_{\text{vHorn.}} = \int d^4x \sqrt{-g} \left[G_4(\phi) R + K(\phi, X) - G_3(\phi, X) \square \phi \right], \quad (2.12)$$

which is also known as the *viable* Horndeski theory [155]. This reduced version of the Horndeski action (2.3) essentially includes the well-known *k*-essence scenario [96, 98, 176–178], the more general Kinetic Gravity Braiding (KGB) theory [40], and a possible non-minimal coupling to gravity *via* the scalar field (see, for instance, reference [154]). In the next sections, we will introduce some of the features of these three types of scalar field theories. For the purpose of this introduction, we will concentrate on examining some general properties in arbitrary backgrounds, leaving the discussion of their specific cosmological applications as DE candidates for the following chapters.

But before continuing any further, we shall emphasise that the action (2.3) represents the most general non-degenerated scalar field theory which features at

¹Alternatively, a dynamical suppression of the GWs speed excess/defect has also been explored in, for instance, references [172, 173].

²Please note that, apart from the conventions related to the signature of the metric and the definition of the kinetic term X in expression (2.8), the cubic term G_3 is also subjected to sign-convention. See different conventions in, for instance, references [2, 40, 174, 175].

most second order field equations. Nevertheless, note that having second order equations is a sufficient but not necessary condition for avoiding the Ostrogradski ghost [102]. Indeed, extensions of the quartic and quintic Horndeski functions, G_4 and G_5 , respectively, have been proposed in references [100, 101]. These scalar models, known as Beyond Horndeski or Gleyzes-Langlois-Piazza-Vernizzi (GLPV) theory, may involve third-order derivatives in the equation of motion of the scalar field when the metric is dynamical, but this does not imply the presence of the Ostrogradski ghost [100]. See also [179] for an earlier example of a scalar theory beyond Horndeski. Moreover, theories with higher-order derivatives whose Lagrangian is degenerated have been also shown to propagate a single scalar DOF and, therefore, they avoid the Ostrogradski ghost [102, 180]. This degeneracy criterion has been used to generalise both Horndeski and Beyond Horndeski into the so-called Degenerated Higher-Order Scalar-Tensor (DHOST) theories [102–104]. The speed of GWs has also been addressed in the context of these extended scalar-tensor theories [181, 182], showing that the region in the parameter space that renders *viable* scalar theories is bigger than that of the viable Horndeski action (2.12) (see also [183] for a discussion on the stability of GWs against decay into dark energy fluctuations in DHOST theories). For the purposes of this thesis, however, we will not address any further the possibility of extending the viable Horndeski family of scalar field theories.

2.2.1 The k -essence scenario

The well-known k -essence theory is given by [96, 98, 176–178]

$$S_g = \int d^4x \sqrt{-g} \left[\frac{1}{2} R + K(\phi, X) \right], \quad (2.13)$$

being K a general function on the scalar field ϕ and its kinetic term X . This represents the most general minimally coupled scalar theory whose action contains up-to first order derivatives of the scalar field. Compared to the viable sub-family of Horndeski theory in equation (2.12), the k -essence scenario corresponds to setting $G_4 \equiv 1/2$ and the braiding function G_3 to zero. (Although a non-zero but constant G_3 would also reduce to the k -essence scenario since the d'Alembertian operator would lead to a boundary term.) This interesting generalisation of the Lagrangian describing a canonical scalar field has been extensively explored in a wide variety of cosmological scenarios, from inflation [96, 97] to DE [98, 176–178].

The field equations follows directly from varying the action w.r.t. to the metric $g_{\mu\nu}$ and the scalar field ϕ . These are [96, 98, 184]

$$G_{\mu\nu} = K_X \nabla_\mu \phi \nabla_\nu \phi + K g_{\mu\nu} + T_{\mu\nu}^{\text{ext}}, \quad (2.14)$$

$$(K_{XX} \nabla^\mu \phi \nabla^\nu \phi - K_X g^{\mu\nu}) \nabla_\mu \nabla_\nu \phi + 2X K_{\phi X} - K_\phi = 0, \quad (2.15)$$

respectively, where $T_{\mu\nu}^{\text{ext}}$ stands for the energy-momentum tensor of the external fields to the action (2.13), such as matter and radiation.

If the derivative of the scalar field is timelike, i.e. when $X > 0$, it is possible to perform a 3+1 slicing of spacetime according to the unit four-vector

$$n_\mu := -\epsilon \frac{\nabla_\mu \phi}{\sqrt{2X}}, \quad (2.16)$$

where $\epsilon := \text{sign}(\dot{\phi})$ ensures that the four-vector is future oriented. Accordingly, co-moving observers with four-velocity n^μ will see the contribution of the scalar field to the right-hand side of equation (2.14) as that of a hydrodynamic fluid (1.3) with energy density and (isotropic) pressure [185]

$$\varrho = 2XK_X - K, \quad (2.17)$$

$$p = K, \quad (2.18)$$

respectively. Moreover, they shall observe a vanishing energy flux q_μ and anisotropic pressure $\pi_{\mu\nu}$. That is [185]

$$q_\mu \equiv 0, \quad (2.19)$$

$$\pi_{\mu\nu} \equiv 0, \quad (2.20)$$

see also previous results in references [186, 187]. Consequently, the contribution of the scalar field as perceived by co-moving observers with four-velocity n^μ is that of a perfect fluid [185].

Due to its simplicity, the k -essence framework has been applied not only in modelling a late-time DE component [98, 176–178], but to inflationary era as well [96, 97]. Nevertheless, this scalar field theory faces several obstacles when considered as a candidate for DE to address the problems of the standard model, most of them inherited from its correspondence with a perfect fluid. As a major challenge, we shall briefly mention that cosmological perturbations suffer from instabilities if the NEC is violated by the scalar field [160, 188–190] (see also reference [1]). Hence, if we interpret the current data as favouring the presence of a slight violation of the NEC in the DE sector at present times [79, 128], a scalar field *à la* k -essence would not provide a robust DE alternative to the cosmological constant. We will further analyse this point in chapter 5. Moreover, these models neither can produce a phantom crossing [191, 192], which was shown to be a necessary prerequisite to ease both the H_0 and S_8 cosmological tensions simultaneously by taking into account new physics relevant only at late cosmic times [131, 132]. Addressing the H_0 tension alone, the k -essence theory was argued to do not perform any better than the standard model [175, 193]. So, with this potential limitations in mind, one may consider the possibility of exploring scalar theories beyond k -essence to produce the desired DE-phenomenology.

2.2.2 Kinetic gravity braiding theory

The KGB theory is given by the action [40] (see also [73, 194])

$$S_g = \int d^4x \sqrt{-g} \left[\frac{1}{2} R + K(\phi, X) - G_3(\phi, X) \square \phi \right], \quad (2.21)$$

which corresponds to setting $G_4(\phi) \equiv 1/2$ in the action (2.12) of the viable Horndeski family. Since only the k -essence function, K , and the cubic function, G_3 , (also dubbed the *braiding* function) appear in the above expression, we will omit hereon the subindex in the cubic function for the sake of the notation, i.e. we will denote $G_3 \equiv G$, when referring to the KGB theory.

The field equations for the metric are [40, 73] (see also reference [158])

$$G_{\mu\nu} = (K_X - G_X \square \phi) \nabla_\mu \phi \nabla_\nu \phi + (K + \nabla_\alpha \phi \nabla^\alpha G) g_{\mu\nu} - 2 \nabla_{(\mu} G \nabla_{\nu)} \phi + T_{\mu\nu}^{\text{ext}}, \quad (2.22)$$

where $G_{\mu\nu}$ is the Einstein tensor and $T_{\mu\nu}^{\text{ext}}$ corresponds to the energy-momentum tensor of the external fields to the action (2.21). When the derivative of the scalar field is timelike, i.e. $X > 0$, the co-moving observer with four-velocity (2.16) see the contribution of the KGB scalar field to the right-hand side of equation (2.22) as that of a hydrodynamic fluid (1.3) with energy density [185]

$$\varrho = 2XK_X - K - 2X(G_\phi + G_X \square \phi) + G_X \nabla_\mu X \nabla^\mu \phi, \quad (2.23)$$

and (isotropic) pressure [185]

$$p = K - 2XG_\phi + G_X \nabla_\mu X \nabla^\mu \phi. \quad (2.24)$$

The scalar field equation, on the other hand, can be cast into the compact form [40, 158]

$$\nabla_\mu J^\mu = p_{,\phi}, \quad (2.25)$$

with

$$J^\mu := (-K_X + G_X \square \phi + 2G_\phi) \nabla^\mu \phi + G_X \nabla^\mu X, \quad (2.26)$$

where $p_{,\phi} = \partial p / \partial \phi$ is the derivative of the pressure w.r.t. the scalar field. The compact form (2.25) will be convenient for later use since it makes transparent the existence of a conserved current (later to be referred to as the shift-current) when p does not depend on the scalar field.

Even though it seems that the second and fourth terms in the current (2.26) would contribute with third-order derivatives to the equation of motion (2.25), these terms appear in the combination $(\nabla_\mu \square \phi - \square \nabla_\mu \phi)$ which can be commuted

away leaving a Ricci tensor coupled to the derivative of the scalar field. Therefore, the scalar field equation (2.25) can be fully expanded as [40]

$$\begin{aligned} L^{\mu\nu}\nabla_\mu\nabla_\nu\phi + (\nabla_\alpha\nabla_\beta\phi)Q^{\alpha\beta\mu\nu}(\nabla_\mu\nabla_\nu\phi) - G_X R^{\mu\nu}\nabla_\mu\phi\nabla_\nu\phi \\ + 2X(K_{\phi X} - G_{\phi\phi}) - K_\phi = 0, \end{aligned} \quad (2.27)$$

where

$$L^{\mu\nu} := (2G_\phi - K_X - 2XG_{\phi X})g^{\mu\nu} + (K_{XX} - 2G_{X\phi})\nabla^\mu\phi\nabla^\nu\phi, \quad (2.28)$$

$$Q^{\mu\alpha\nu\beta} := (g^{\mu\alpha}g^{\nu\beta} - g^{\mu\nu}g^{\alpha\beta})G_X - (g^{\mu\alpha}\nabla^\nu\phi\nabla^\beta\phi - g^{\mu\nu}\nabla^\alpha\phi\nabla^\beta\phi)G_{XX}. \quad (2.29)$$

From the expanded version in equation (2.27) it is clear that no derivatives higher than second-order appear, thus the Ostrogradski instability does not apply. Moreover, $\ddot{\phi}$ enters only linearly in equation (2.27) due to the structure of the tensor $Q^{\mu\alpha\nu\beta}$, which is sufficient to ensure that the Cauchy problem has a unique local solution, provided that the functions K and G are sufficiently smooth [40]. Another important property of the KGB theory is that second-order derivatives of the scalar field are present in the metric equation of motion (2.22) when G_X is not trivial, and vice versa. Second-order derivatives of the metric enter the equation of motion of the scalar field (2.27) due to the Ricci tensor. Therefore, the system (2.22) and (2.27) is non-diagonal in second derivatives when G_X is not trivial. This is a direct manifestation of the *kinetic braiding* due to the d'Alembertian operator in the KGB action (2.21) and leads to a number of interesting features.

For general configurations with timelike field derivatives, the presence of the d'Alembertian operator makes the energy-momentum tensor not to coincide with that of a perfect fluid as seen by co-moving observers with four-velocity (2.16). This is because, contrary to k -essence, the energy flux vector [185]

$$q_\mu = -\frac{G_X}{\sqrt{2X}}\left(2X\nabla_\mu X + \nabla_\alpha X\nabla^\alpha\phi\nabla_\mu\phi\right), \quad (2.30)$$

is, in general, non-zero (see also [41]); whereas the anisotropic pressure $\pi_{\mu\nu}$ is always trivial [185]. The perfect fluid approximation can be, nevertheless, safely assumed for highly symmetric backgrounds [40] (see also [185, 195]). This is precisely the case of the FLRW metric. However, small deviations from the cosmological solution cannot be addressed as those produced by a perfect fluid [41, 194]. As a result, the *imperfect* nature of the KGB-fluid allows for features otherwise not possible for a theory with a single minimally coupled scalar field *à la* k -essence [41]. Being the most remarkable examples the possibility of a stable violation of the NEC in the dark sector or producing a phantom crossing [40, 41].

Due to their interesting properties, the KGB models have been widely explored in the context of both early- and late-time cosmology; see, for instance, applications to inflation in references [96, 158, 196–198] and DE models [40, 168, 189, 199–207]. In addition, the parameter-space of the theory has also been confronted with cosmological observables [208–212], rendering this set-up as a plausible DE model. Nevertheless, note that some specific subclasses of the KGB theory may be found in tension with cosmological data (see, for example, the discussion on Cubic Galilean gravity in references [213–215]). The KGB set-up has also been studied in the context of the H_0 tension, showing a possible modest increase in the value of H_0 in these theories [175]. Moreover, the Palatini version of the KGB theory and its connection to the metric formalism have been previously explored in reference [216].

In chapter 4 we discuss the expansion history of a flat FLRW background in the KGB theory. We re-obtain the well-known de Sitter (dS) future solutions using a novel dynamical systems analysis. Moreover, we also discuss the occurrence of cosmological singularities. In fact, we present new examples where the evolution of the system inevitably approaches a big rip [88, 217], a big freeze [218, 219] or a sudden singularity [220, 221]. To best of our knowledge, this is the first time these singular behaviours are discussed in the context of the KGB theory. In chapter 5, we focus on the stability of the KGB theory from the point of view of scalar perturbations.

2.2.3 Metric $f(R)$ theories of gravity

The metric $f(R)$ theory of gravity³ come about as a straightforward generalization of the Einstein–Hilbert action for the gravitational sector in which the scalar curvature has been replaced by a arbitrary function of R . That is [222]

$$S_g = \frac{1}{2} \int d^4x \sqrt{-g} f(R), \quad (2.31)$$

where different choices for the function f leads to different gravity theories. Note that GR corresponds to the case of $f(R) = R$.

These types of modified theories of gravity were first proposed in the 70s [222], but later they gained more attention in the context of inflation [223, 224] and, more recently, as DE candidates [225–228] (see also references [110, 229] for a modern review). The equations of motion can be obtained, in the metric approach, from varying the action (2.31) w.r.t. the metric. This leads to [224, 229–231]

$$f_R R_{\mu\nu} - \frac{1}{2} f g_{\mu\nu} - (\nabla_\mu \nabla_\nu - g_{\mu\nu} \square) f_R = T_{\mu\nu}^{\text{ext}}, \quad (2.32)$$

being $T_{\mu\nu}^{\text{ext}}$ the energy-momentum tensor associated to the external sources to the gravitational action (2.31) as commonly defined in, for instance, equation (1.10). Note that the metric field equations (2.32) are, generally, of fourth-order, whereas Einstein's equations (1.2) remain second-order. This structure implies the existence of an additional DOF to those already propagated in GR. Indeed, the linearised spectrum of the theory has been shown to be that of the usual GR's graviton plus a scalar field [232]. Moreover, this new DOF in metric $f(R)$ trivially evades the Ostrogradski instability, as we discuss below. The interested reader may find an insightful discussion on the general features of $f(R)$ gravity in, for instance, references [224, 233].

The new scalar DOF in the theory can be made explicit by invoking an auxiliary field, χ , that obeys the action [230] (see also references [224, 229])

$$S_g = \frac{1}{2} \int d^4x \sqrt{-g} \left[f(\chi) + f_\chi(\chi)(R - \chi) \right]. \quad (2.33)$$

Varying the above expression w.r.t. the auxiliary field χ leads to

$$f_{\chi\chi}(R - \chi) = 0, \quad (2.34)$$

from where it follows $R = \chi$ provided that $f_{\chi\chi} \neq 0$ [224, 229, 230]. Taking this solution into account, the form of action (2.33) reduces to that of the original action of $f(R)$ gravity given in expression (2.31): they are dynamically equivalent [224, 229, 230]. Finally, the new scalar field (dubbed “scalaron” [223]) is made explicit in the theory by defining

$$\phi := f_\chi(\chi), \quad (2.35)$$

in the action (2.33). It follows then that the original $f(R)$ action (2.31) is equivalent to [224, 229, 230]

$$S_g = \frac{1}{2} \int d^4x \sqrt{-g} \left[\phi R - V(\phi) \right], \quad (2.36)$$

where

$$V(\phi) = \chi(\phi)\phi - f(\chi(\phi)), \quad (2.37)$$

³In the metric version of the theory, the connection $\Gamma_{\beta\gamma}^\alpha$ is considered to be totally determined by the metric $g_{\mu\nu}$. Thus, the metric $g_{\mu\nu}$ is the only independent variable for the variational procedure. In other approaches, like Palatini or metric-affine $f(R)$ gravity, the metric and the connection are assumed to be independent variables and, therefore, the corresponding action is varied w.r.t. both of them. The difference between the Palatini and metric-affine approaches lies in the additional assumption that the (external) matter fields do not depend on the connection in the former formalism, whereas this condition is relaxed in the latter [224]. In general, these variational formalisms lead to non-equivalent equations of motion; see, for example, reference [224]. Here we will only consider the metric version of the theory.

is a potential-like term for the scalar field ϕ . In this way, the metric version of $f(R)$ gravity can be re-formulated as a scalar-tensor theory. Moreover, a direct comparison of action (2.36) with expression (2.12) reveals that these modified theories of gravity belong to the viable subclass of Horndeski gravity [224, 229], where

$$G_4(\phi) = \frac{\phi}{2}, \quad K(\phi) = -\frac{V(\phi)}{2} \quad \text{and} \quad G_3 \equiv 0, \quad (2.38)$$

which also corresponds to a Brans-Dicke theory with $\omega \equiv 0$ [232, 234]. A straightforward result of this comparison is that these theories are free from the Ostrogradski's ghost and GWs are propagated luminically. In fact, it seems that $f(R)$ is unique among other higher-order Ricci-based modifications to gravity as it is the only known scenario that trivially avoids the Ostrogradski instability [224].

Please note that the absence of a kinetic term for the scalar field in the above action does not imply that the extra scalar DOF is non-dynamical. Its evolution is due to the non-minimal coupling to the scalar curvature (see, for instance, [224]). In Einstein's frame, however, this non-minimal coupling may introduce a fifth-force effect due to the exponential coupling of the scalar to the matter fields [235]. Since fifth forces have not been so far detected in either ground-based or Solar System experiments, these types of modification to gravity are in general disfavoured observationally [236–242] (see also reference [235]). Nevertheless, a screening mechanism based on the *Chameleon* effect can be invoked to reconcile some $f(R)$ models with local experiments [243–245]. See also references [246–251] for an interesting discussion on reliable $f(R)$ candidates that evade these low-curvature-regime tests.

In chapter 6 we discuss the possibility of modelling the accelerated expansion in the framework of $f(R)$ theories of gravity. Moreover, we examine how to reproduce a given DE effective EOS in metric $f(R)$ gravity. To that aim, we take some phantom-DE models in FLRW that have been already observationally constrained and obtain their asymptotic $f(R)$ versions. Then, we analyse the occurrence of phantom singularities in both the classical and quantum regime of the modified theory of gravity.

2.3 Shift symmetry for the dark sector

One of the arguments most commonly used to go beyond the standard model of cosmology is the existence of a fine-tuning problem regarding the value of the cosmological constant [24, 25]. Scalar field theories have long been studied to see if they could alleviate some of this fine-tuning problem [24, 157, 252–254] (see also the reviews [77, 255]). The main idea is to produce a sort of self-adjustment

mechanism such that the effective vacuum energy density gets screened away or nearly cancelled when the system reaches equilibrium [24, 25] (see also reference [256] for a similar discussion with a massless vector field). Nevertheless, Weinberg’s no-go theorem [24] shows under general assumptions that such mechanism cannot completely screen any vacuum energy without re-introducing a fine-tuning dilemma now related to the parameters describing the equilibrium configuration of the scalar field (see also [77] for a review on the theorem). It may seem, therefore, that such mechanism cannot in practice contribute to the resolution of the original problem. However, as highlighted by Weinberg himself, this no-go theorem restricts but does not close-off all hope in this direction [24].

Scalar field models able to consistently screen-out any vacuum energy were first proposed by Charmousis et al. [157, 253] via relaxing one of Weinberg’s assumptions (see also, e.g., reference [257]). By construction, these models lead to a future Minkowski state for any kind of material content at which the scalar field retains a non-trivial time dependence. Moreover, the screening is robust in the sense that the final Minkowski state does not depend on the precise matter content or the initial conditions. However, a late-time accelerating phase does not naturally arise in these models [254]. For this reason, the self-adjustment idea was later extended from Minkowskian to dS final states [202, 203, 258, 259]. In addition to these considerations, we shall also highlight that scalar field theories where the contribution of the scalar field to the total energy density mimics the scaling of the dominant component (known as *scaling* or *tracker* solutions [260, 261]) have been discussed in the context of their future dS attracting solutions [201, 262] and the coincidence problem [263, 264].

A general problem⁴ of scalar theories, however, is that having potential-like terms could reintroduce the fine-tuning problem now regarding the parameters that fix the minimum of the potential at the equilibrium point, if the accelerated expansion is reached in the potential domination regime. One possible way of trying to avoid this problem is the consideration of a shift-symmetric scalar field, which guarantees that the cosmic acceleration is driven by the kinetic energy [201, 265]. These are scalar theories that are invariant under constant shifts in the scalar field, namely

$$\phi \rightarrow \phi + c, \tag{2.39}$$

for which potential-like terms do not appear in the Lagrangian. This symmetry-based argument is an elegant way to make the evolution of the system to depend only on the rate of change of the scalar field but not on the scalar field itself. Moreover, the absence of a potential-like terms is also protected against radiative corrections if this symmetry is maintained at the quantum level. On a more

⁴Related to some extent to Weinberg’s no-go theorem.

practical side, it is also important to highlight that the existence of a global symmetry leads to a conserved quantity. This conserved quantity can in fact be used to reduce the order of the original background equations, thus, simplifying the mathematical treatment of the model. We will comment more on this in chapters 4 and 5 when analysing the shift-symmetric version of the KGB theory. In the literature, this symmetry has been extensively explored in a great variety of scenarios including, for instance, inflation [73, 96, 158, 266], late-time cosmology [40, 200, 203, 204, 254] and black hole physics [267, 268].

When applied to the viable Horndeski subclass (2.12), the shift-symmetry forces the free functions to do not depend on ϕ . In particular, this makes the non-minimal coupling function G_4 to take a constant value. As a result, the $f(R)$ theory of gravity in its scalar field representation is practically ruled out by this symmetry argument. Within the remaining models, the shift-symmetric version of the KGB theory will play a central role in the main part of this thesis. Thus, in chapter 4 we will discuss the background evolution of these shift-symmetric scalar field theories. In chapter 5 we will focus on the stability of the theory from the point of view of scalar perturbations.

2.4 Dynamical systems analysis

Dynamical systems provide an interesting framework for extracting qualitative information about the behaviour of a given cosmological model. Within this approach, we construct a configuration space associated to the original background equations and study the structure of the flow that drives the evolution of the selected variables. The points in the configuration space where the flow vanishes provide us with valuable information about the different phases in the evolution of a given cosmological model. It should be pointed out, nevertheless, that this analysis does not reveal any quantitative information about the precise time evolution of the original model, for which the background field equations must be solved. In this section, we briefly introduce the terminology and techniques to be used later in chapter 4 when analysing the background evolution of the KGB theory.

Let be $\mathbf{x} = (x_1, \dots, x_n) \in \mathbb{S}$ an element of the space $\mathbb{S} \subseteq \mathbb{R}^n$. A dynamical system is usually expressed as [269, 270]

$$\mathbf{x}' = \mathbf{f}(\mathbf{x}), \quad (2.40)$$

where a prime denotes derivation w.r.t. a suitable time-like (affine) parameter and where the function $\mathbf{f} : \mathbb{S} \rightarrow T_{\mathbf{x}}\mathbb{S}$ given by

$$\mathbf{f}(\mathbf{x}) = (f_1(\mathbf{x}), \dots, f_n(\mathbf{x})), \quad (2.41)$$

can be interpreted as a vector field that is tangent at each point $\mathbf{x} \in \mathcal{S}$ to the trajectory, i.e. the solution curve to the equations (2.40), passing through that point [269, 270]. The proper construction of the configuration space \mathcal{S} and the system (2.40) in cosmology will be addressed in chapter 4 for the KGB theory. The reader may find further information on dynamical systems and their applications to different cosmological models in references [271–279]; see also the cornerstone books [269, 270, 280] for a more technical treatment.

The first important notion in dynamical systems is that of the *fixed points* of the system (2.40).

Fixed point A fixed point, also known as critical point or equilibrium point, is a point $\mathbf{x}_0 \in \mathcal{S}$ at which $\mathbf{f}(\mathbf{x}_0) = 0$. According to (2.40), these points represent steady states where the system is at rest in the configuration space.

In principle, the system could remain in this equilibrium state indefinitely. However, it is important to assess whether or not the system will remain at these configurations when subjected to small perturbations around them. For the scope of this thesis, it will be enough to discuss the linearised version of the system (2.40) to understand the stability of the whole system around that a given fixed point. In this approach, the Jacobian matrix

$$\mathcal{J}(\mathbf{x}_0) = \frac{\partial f_i}{\partial x_j} \Big|_{\mathbf{x}_0} = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} \Big|_{\mathbf{x}_0} & \cdots & \frac{\partial f_1}{\partial x_n} \Big|_{\mathbf{x}_0} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_n}{\partial x_1} \Big|_{\mathbf{x}_0} & \cdots & \frac{\partial f_n}{\partial x_n} \Big|_{\mathbf{x}_0} \end{pmatrix}, \quad (2.42)$$

plays a central role as it contains all the information about the first order Taylor expansion of $\mathbf{f}(\mathbf{x})$ around \mathbf{x}_0 . Indeed, the stability of a given fixed point in the linearised system coincides with that of the non-linear system if the Jacobian matrix has no eigenvalues with zero real parts (see the Hartman–Grobman theorem in, for instance, references [269, 270]). This motivates the following classification of the fixed points according to the validity of the linear approach.

Hyperbolic fixed points These are isolated critical points at which all the eigenvalues of the Jacobian matrix (2.42) have non-zero real parts. Therefore, the linearised analysis is sufficient to address their stability.

Normally hyperbolic fixed points This is a set of non-isolated equilibrium points for which the only eigenvalues of the Jacobian matrix (2.42) with zero real parts are those whose corresponding eigenvectors are tangent to the set containing the equilibrium points. The stability of these non-isolated fixed points can be addressed within the linear theory restricted only to the eigenvalues with non-trivial real parts [270, 280].

Non-hyperbolic fixed point These are isolated critical points at which (at least) one of the eigenvalues of the Jacobian matrix (2.42) has a zero real part. Linear stability theory fails for these points and more advanced techniques like Centre Manifold Theory or Lyapunov’s method should be used [269] (see also references [273, 275, 277, 278]).

Non-hyperbolic fixed point will not appear in our analysis in chapter 4 and, therefore, we will not discuss them any further. In the following, we will focus on the linear stability of (normally) hyperbolic equilibrium points. According to the linearised theory, the stability of these configurations depends only on the real parts of the eigenvalues associated to the Jacobian matrix [269]. The different possibilities are listed below⁵.

Attractors These are (normally) hyperbolic critical points at which the (non-zero) real parts of the eigenvalues of the Jacobian matrix (2.42) are all negative. These represent stable configurations. In the configuration space, nearby trajectories converge to these fixed points.

Repellers These are (normally) hyperbolic critical points at which the (non-zero) real parts of the eigenvalues of the Jacobian matrix (2.42) are all positive. These represent unstable configurations. In the configuration space, nearby trajectories depart from these fixed points.

Saddle points These are (normally) hyperbolic critical points that are neither attractors nor repellers. The Jacobian matrix (2.42) has eigenvalues with both positive and negative real parts. In the configuration space, some trajectories may come arbitrarily close to these equilibrium points, as they feel attracted from some directions and repelled along others.

The study of the unstable (repellers) and stable (attractors) equilibrium points is a useful approach to the cosmological evolution of a given model since trajectories in the configuration space usually evolve from the former to the latter equilibrium points; these are called *heteroclinic* orbits [269, 270, 280]. Moreover, the existence of saddle configurations also gives valuable information about intermediate phases in the expansion history; note, for instance, the matter-dominated epoch in Λ CDM. These characteristics make dynamical systems analysis an interesting tool to scrutinise the possible phenomenology of different DE models. Nevertheless, the dynamical system approach only provides qualitative information about the would-be solution to the background equations. Therefore, the

⁵Here we do not discuss the subtle difference between stable/unstable and *asymptotically* stable/unstable critical points [269] since all the fixed points we will study belong to the latter group.

information obtained from this technique must be combined with a close inspection of the background equations themselves to obtain as much information as possible on the whole evolution of the system.

2.5 Dark energy fluctuations

Contrary to the cosmological constant case, a dynamical DE may introduce a new DOF that should be properly taken into account when computing the cosmological perturbations. The stability conditions for a dynamical DE model can be obtained by isolating the new propagating DOF and analysing its Lagrangian (see, for instance, references [281–283]). In this section we review the main stability criteria for the description of linear perturbations around a flat FLRW background. We focus on the scalar sector only since the KGB theory (for which we will later discuss the stability) does not alter the tensor sector at linear order. It is worth saying, however, that the instabilities discussed below may also appear for the vector and tensor modes in more general scalar theories. The viability conditions for the Horndeski theory has been thoroughly analysed in references [168, 284].

In order to introduce the main criteria for the stability of linear scalar perturbations, we shall consider here a single scalar DOF propagating around a flat FLRW background. This is an oversimplification since the perturbations of the matter content of any physically reasonable model of the cosmos will also contribute to the scalar sector. Nevertheless, this simplification will come in handy for introductory purposes, whereas a more realistic scenario may be found in reference [168]. In general, linear order scalar perturbation around a flat FLRW background can be described by the second-order action

$$S_{\text{scalar}}^{(2)} = \int d^4x a^3 \left\{ Q_S \left[\dot{u}^2 - \frac{c_s^2}{a^2} (\nabla_i u)^2 \right] - m_{\text{eff}}^2 u^2 \right\}, \quad (2.43)$$

where the dot represents time derivation, ∇_i is the spatial gradient and u denotes the corresponding scalar perturbation. The quantities Q_S , c_s^2 and m_{eff}^2 can, in general, depend on the background time t and they play a central role in the characterization of the stability of the theory.

For general time-dependent coefficients Q_S , c_s^2 and m_{eff}^2 like in action (2.43), there is no clear definition for the stability of the solutions for $u = u(t, x)$ [285]. However, in the limit where the time and length scales considered are much shorter than the rate of variation of the background, it is perfectly acceptable to analyse the stability of the system as if the quantities Q_S , c_s^2 and m_{eff}^2 were constant at a given time [285] (see also reference [286]). Within this *local* approximation to the stability of the theory, the background will be stable (against scalar perturbations)

provided that the three previously mentioned quantities are positive [190]. That is,

$$\text{Healthy background: } Q_s > 0, \quad c_s^2 \geq 0 \quad \text{and} \quad m_{\text{eff}}^2 \geq 0. \quad (2.44)$$

Different types of instabilities may appear if any of these conditions are violated, which are related to the change in the global and/or relative signs between the different terms in action (2.43). In the following, we review the main instabilities discussed in the literature, and their physical interpretation. For the sake of the presentation, we will discuss the violation of the above inequalities one by one. However, more than one of these conditions may be violated at the same time in a real situation, leading to the simultaneous presence of several instabilities.

Gradient instability Also known as Laplacian instability, it appears when the leading order spatial derivatives have the wrong sign w.r.t. the time derivatives in the perturbed action [190] (see also references [287]). In the proxy action (2.43), this instability can be avoided by demanding that [190]

$$c_s^2 \geq 0, \quad (2.45)$$

where c_s^2 plays the role of the speed of propagation (hereon referred to as the *speed of sound*) of the scalar perturbation u . If the above condition is satisfied, the corresponding field equation for $u(t, x)$ is of hyperbolic form, which features wave-like solutions. Conversely, the structure of this differential equation changes from hyperbolic to elliptic if c_s^2 is negative. As a result, the frequencies of the oscillations become imaginary (at least) at high momenta, which produces perturbations that grow exponentially fast in Fourier space. Thus, it precludes a stable classical model (at least, as long as a perturbative treatment is still valid). The characteristic timescale of this instability is directly proportional to the wavelength. Hence, this instability is particularly dangerous for short-wavelength modes [155]. For a more involving situation than the one described by the proxy action (2.43), where more than one scalar mode is present or the action is not diagonal in the time and spatial derivatives, the presence of this stability can be addressed by analysing the corresponding dispersion relations, where it should be ensured that the resulting frequencies are always real at high momenta [285].

Ghost instability This is when the kinetic energy of the background perturbations is negative. In the proxy action (2.43), the ghost instability is avoided provided that [190]

$$Q_S > 0. \quad (2.46)$$

In Fourier space, the no-ghost condition is manifestly k -independent for the Horndeski theory [168, 210, 284]. However, a dependence on the momenta of the mode

may appear in more general scalar field theories [288]. In that situation, a ghost-like instability is usually defined only in the large- k regime [210, 287, 288], whereas low-momenta ghosts have been argued to be harmless [288]. Indeed, these infrared ghosts were shown to be related to the physical phenomenon of a tachyon/J Jeans instability, which we discuss below [289]. From a physical point of view, if the ghost-free condition is violated there may be runaway solutions (at the classical level) when the ghost DOF interacts with a positive energy mode. These are classical solutions where the total energy is conserved while individual energies associated to the ghost and no-ghost sectors diverge; we referred the interested reader to the discussion in, for example, reference [290]. Thereby, the common lore states that ghost instabilities are catastrophic (already) at classical level. Still, the classical background is stable against high momenta perturbations [190]. Contrary to this common conception, it should be noted that there are examples in the literature in which the presence of a ghost DOF interacting with a positive energy DOF do not lead to runaway solutions and, therefore, to the destabilization of the classical motion of the system [291]. (See also *islands of stability* [292, 293] and *meta-stability* of ghosts [294, 295].) Upon canonical quantisation of theories with ghosts, the energy conservation does not forbid pair creation from vacuum of ghosts-particles together with normal-particles: the vacuum becomes quantum mechanically unstable (see, for instance, references [190, 290]). So, the presence of a ghost is also considered to be pathological at the semi-classical level. However, the possibility of safely living with ghosts at the quantum level has already been explored with positive conclusions; e.g. references [296–305] (see also references [306, 307] for applications to quadratic gravity).

Tachyon and Jeans instability Less addressed than the ghost and gradient instabilities, the tachyon instability appears as the effective squared mass in action (2.43) becomes negative. This forces the frequencies of the oscillations to become imaginary at low momenta, which results in an exponentially growing perturbation. Contrary to the gradient instability, the timescale over which this instability develops is given by the inverse of the effective mass in the long wavelength limit and, therefore, it is independent of the momenta [71, 308]. The Hamiltonian can be shown to be unbounded from below at low momenta [287]. Thus, this instability was also referred to as infrared ghosts in some references [289]. Nevertheless, it should be clear that the physical implications of a ghost or a tachyon instability are very different [288, 289]. The tachyon instability can be avoided provided that [190]

$$m_{\text{eff}}^2 \geq 0, \quad (2.47)$$

in the proxy action (2.43). However, it is also possible to have $m_{\text{eff}}^2 < 0$ without producing exponential modes for certain length and time scales. That is when

the negative squared-mass is compensated by the usual momentum contribution, proportional to $c_s^2 k^2$, to the dispersion relation so that the resulting frequencies are real for $k > k_J$, where k_J is the critical wavenumber [309, 310]. For modes with momenta lower than k_J (wavelength bigger than the critical scale), frequencies become imaginary and, therefore, the perturbation grows. This behaviour is known as Jeans instability, and it plays a crucial role in our understanding of how large-scale structures form in the universe [309, 310].

It is important to highlight that in the case of the timescale at which the instability develops being comparable to the characteristic timescale at which the background evolves, the approximation of Q_S , c_s^2 and M_{eff}^2 as slowly varying quantities cannot be trusted. In such situation, a full stability analysis of the complete set of perturbed background equations will be required. Finally, we should briefly mention that the above listed instabilities are not the only possible concerns for the viability of a given theory. Indeed, superluminal propagation and causality-related issues may also restrict the viable parameter-space of the theory. However, we will not address these possible issues here (see, for instance, references [71, 159]). In chapter 5 we will discuss the viability of the KGB theory from the point of view of the stability of the corresponding linear-order scalar perturbation.

2.6 Effective field theory of dark energy

The framework of EFT will be also useful for addressing the cosmological perturbations up-to arbitrary order. Therefore, in this section we revise the main ideas and key concept behind this approach.

This framework was first applied to DE in reference [160] (see also [311, 312] for applications to inflationary models) and further developed in references [174, 313–315] (see also reference [287] for a review). This approach considers the most general form for the gravitational action (including cosmological perturbations up-to an arbitrary order) built-up only on symmetry arguments. Originally, this framework was based on two assumptions [174]: *i*) the validity of the weak equivalence principle and the existence of a Jordan metric $g_{\mu\nu}$ universally coupled to matter fields; *ii*) the existence of a unitary gauge compatible with the residual symmetries of the unbroken spatial diffeomorphisms.

The last of these assumptions advocates for the presence of a scalar field in the DE sector. This is because the presence of a homogeneous scalar field $\phi(t)$ in a FLRW background defines a preferred time slicing of spacetime. These are the hypersurfaces with ϕ constant and, therefore, $\delta\phi \equiv 0$ on them. So, for this choice (unitary gauge) only metric degrees of freedom are explicitly displayed in the action. The scalar field perturbation can be reintroduced explicitly in the theory

via the Stückelberg trick. That is, by performing infinitesimal time diffeomorphism $t \rightarrow t + \pi(t, x)$ being π the scalar field fluctuations; see appendix E. However, in this approach π does not represent the original scalar field ϕ in the DE sector, but the perturbations encoding the scalar degree of freedom in the theory.

In order to construct the most general expression for the action satisfying the previous ansätze, note that hypersurfaces with constant ϕ can be defined as those orthogonal to the unit four-vector (2.16), provided that $\partial_\mu \phi$ is time-like, i.e. $X > 0$. (Here we are not going to consider oscillating solutions where the background field velocity, $\dot{\phi}$, crossed zero since this case may be problematic in standard perturbation theory [194].) For a homogeneous scalar field, that is $\phi = \phi(t)$, this four-vector reduces to

$$n_\mu = -\frac{\delta_\mu^0}{\sqrt{-g^{00}}}. \quad (2.48)$$

This slicing induces the spatial metric

$$h_{\mu\nu} = g_{\mu\nu} + n_\mu n_\nu, \quad (2.49)$$

where $n_\mu n^\mu = -1$ and $n^\mu h_{\mu\nu} = 0$. Physically, h_μ^ν represents the projector that leads, at each point of the spacetime, to the rest space of a co-moving observer with four-velocity n^μ [316].

Note that invariance under time-translations is spontaneously broken (in the sense discussed in reference [315]) since the scalar field signals out a preferred time. The terms allowed in the EFT action are, therefore, those invariant under the residual symmetries of the unbroken spatial diffeomorphisms, such as the contravariant time-time component of the Jordan metric g^{00} . The extrinsic curvature of constant time hypersurfaces is also allowed to appear. This is defined as [38]

$$\mathcal{K}_{\mu\nu} := h_\mu^\alpha \nabla_\alpha n_\nu, \quad (2.50)$$

and represents the spatial projection of the covariant derivative of n_ν . (Note that the extrinsic curvature is sometimes defined with a different sign convention, see, for instance, references [110, 196].) In addition, its trace reads

$$\mathcal{K} = \nabla_\mu n^\mu. \quad (2.51)$$

The Ricci scalar R , any curvature invariants, and contractions of tensors with $g_{\mu\nu}$, n_μ and the covariant derivative ∇_μ are also invariant under spatial diffeomorphisms. Therefore, the most general EFT action can be expressed as [311]

$$S_g = \int d^4x \sqrt{-g} \mathcal{L}(R_{\mu\nu\rho\sigma}, \mathcal{K}_{\mu\nu}, g^{00}, t), \quad (2.52)$$

where time is also allowed to appear explicitly. For addressing the cosmological perturbation, however, it is more convenient to split the above action into two parts. The first one contains all the terms that affect the background. Hereon, we will refer to this group as the *background* terms. The second part encompasses all the quantities that only affect the dynamics of the perturbations (at any order). In this way, the above action can be recast in the form of [174] (see also [311, 314])

$$S_g = \int d^4x \sqrt{-g} \left[\frac{M_*^2}{2} f(t) R - \Lambda(t) - c(t) g^{00} \right] + S_{DE}^{(2)}, \quad (2.53)$$

where f , Λ and c are functions of time. Moreover, the latter two background quantities read

$$c = \frac{M_*^2}{2} (-\ddot{f} + H\dot{f}) + \frac{1}{2} (\varrho_{DE} + p_{DE}), \quad (2.54)$$

$$\Lambda = \frac{M_*^2}{2} (\ddot{f} + 5H\dot{f}) + \frac{1}{2} (\varrho_{DE} - p_{DE}), \quad (2.55)$$

being p_{DE} and ϱ_{DE} the pressure and energy densities of the DE fluid. In addition, M_*^2 is the Planck mass, which in the geometric unit system we have adopted here it is equal to one. Conversely, $S_{DE}^{(2)}$ contains all terms that start at quadratic order in perturbations and, therefore, they do not affect the background. (Recall, however, that the background quantities do influence the perturbative behaviour.) This part can be expressed as follows [174]

$$\begin{aligned} S_{DE}^{(2)} = \frac{1}{2} \int d^4x \sqrt{-g} & \left[M_2^4 (\delta g^{00})^2 - \bar{m}_1^3 \delta g^{00} \delta \mathcal{K} - \bar{M}_2^2 \delta \mathcal{K}^2 - \bar{M}_3^2 \delta \mathcal{K}_\mu{}^\nu \delta \mathcal{K}_\nu{}^\mu \right. \\ & + m_2^2 h^{\mu\nu} \partial_\mu g^{00} \partial_\nu g^{00} + \lambda_1 \delta R^2 + \lambda_2 \delta R_{\mu\nu} \delta R^{\mu\nu} + \mu_1^2 \delta g^{00} \delta R + \gamma_1 C^{\mu\nu\rho\sigma} C_{\mu\nu\rho\sigma} \\ & \left. + \gamma_2 \epsilon^{\mu\nu\rho\sigma} C_{\mu\nu}{}^{\kappa\lambda} C_{\rho\sigma\kappa\lambda} + \frac{M_3^4}{3} (\delta g^{00})^3 - \bar{m}_2^3 (\delta g^{00})^2 \delta \mathcal{K} + \dots \right], \quad (2.56) \end{aligned}$$

where M_i^4 , \bar{M}_i^2 , m_i^2 , \bar{m}_i^3 , λ_i and γ_i are the parameters of the theory, and the ellipsis stand for additional third order operators which can be included, e.g. $\delta \mathcal{K}^3$. Generally, all these parameters are allowed to depend on the time coordinate t . The quantities M_i^4 , \bar{M}_i^2 , m_i^2 , \bar{m}_i^3 and μ_i are commonly called *mass parameters* [174]. In addition, $\delta g^{00} := g^{00} + 1$ is the perturbation of the metric, $\delta \mathcal{K}_\nu{}^\mu$ is the perturbation of the extrinsic curvature, and $\delta \mathcal{K}$ the perturbation of its trace. Likewise, $\delta R_{\mu\nu}$ is the perturbation of the Ricci tensor and δR the perturbation of its trace, whereas $C_{\mu\nu\rho\sigma}$ represents the Weyl tensor defined as [290, 317]

$$C_{\mu\nu\rho\sigma} := R_{\mu\nu\rho\sigma} - (g_{\mu[\rho} R_{\nu]\sigma} - g_{\nu[\rho} R_{\mu]\sigma}) + \frac{R}{3} g_{\rho[\mu} g_{\nu]\sigma}. \quad (2.57)$$

The reason why this tensor appears in the above action instead of the perturbations of the Riemann tensor, namely $\delta R_{\mu\nu\rho\sigma}$, as may be expected is simple. Since the FLRW metric is conformally flat (for $k = 0, \pm 1$), the Weyl tensor automatically vanishes on the background [312] (see also references [318, 319]). Owing to the above relation, we can use the Weyl tensor instead of the perturbed Riemann since the former already starts at first order in perturbation theory.

The action (2.56) describes a great variety of DE models encompassing a single scalar DOF [174]. Please note that the expansion in expression (2.56) sets two different scales: one related to the number of perturbations, other related to the number of spatial derivatives. Thus, some operators like M_2^4 modifies only the normalisation of the perturbation (no spatial derivatives involved), others contribute to the usual linear dispersion relation (two spatial derivatives involved). Operators like \bar{M}_2^2 and \bar{M}_3^2 , on the other hand, introduce modifications to the dispersion relations since they are second order in perturbations but they contain more than two spatial derivatives [314, 315]. The EFT action (2.56) does not represent, however, theories like massive gravity away from the decoupling limit [174]. Different couplings to the dark matter sector can also be included in this effective description with minor modifications [174]. Additional operators should also be included [320] to describe the new found DHOST theories [102, 180]. The same holds for Lorentz violating theories [161, 321] like Hořava-Lifshitz gravity [322, 323].

3

The fate of the Universe

DARK ENERGY is the dominant component in the Universe today. Moreover, at least for the most common models that we have, this dark component stays constant or dilutes slower than matter with the expansion. Hence, DE will be even more dominant in the future. Unravelling the nature of this mysterious component will, therefore, provide a hint to the possible future (classical) evolution of the universe.

In the standard Λ CDM model, the cosmological constant plays the role of DE. As normal matter dilutes with the expansion, this constant drives the Universe to a final dS state characterized by an exponential expansion

$$a(t) \propto e^{\sqrt{\Lambda/3}t}, \quad (3.1)$$

where Λ is the cosmological constant. Deviation w.r.t. this constant in the modelling of DE will possibly lead to a very different future evolution, from future vacuum states if DE is quintessence-ish to cosmological singularities in the case of some phantom energy. Thus, the future evolution of the universe strongly depends on the nature of the DE sector. It is worth mentioning, however, that depending on the predictions of the classical model, quantum corrections may arguably be required. This is because the prediction of any singularity could indicate the breakdown of the classical theory. However, in some cases, it may be possible to extend the dynamics beyond the singular region; see, for instance, references [324–327] and references therein.

In this chapter we delve into the consequences of DE being of a phantom nature. Hence, we start by reviewing the very concept of phantom energy in section 3.1. The definition and classification of cosmological singularities are introduced in section 3.2. Finally, we comment in section 3.3 on the treatment of classical singularities in the framework of quantum cosmology.

3.1 Phantom energy

So far, we have repeatedly mentioned the possibility of having a *phantom* regime in cosmology. Here we comment in more detail the properties and possible issues that such phase would have from the point of view of an effective fluid description.

A phantom fluid is an exotic form of energy with positive energy density and very strong negative pressure such that not only the SEC is violated, but the NEC as well [59]. That is,

$$\varrho_{\text{ph}} + p_{\text{ph}} < 0, \quad (3.2)$$

being ϱ_{ph} and p_{ph} the (effective) energy density and pressure of the phantom fluid. As a result, the EOS parameter of phantom energy,

$$w_{\text{ph}} := \frac{p_{\text{ph}}}{\varrho_{\text{ph}}}, \quad (3.3)$$

is less than -1. Contrary to *normal* matter, the covariant conservation of the energy-momentum associated to the phantom fluid implies that the energy density of phantoms increases with the cosmic expansion [59]. On a FLRW background, this reads

$$\dot{\varrho}_{\text{ph}} = -3H(\varrho_{\text{ph}} + p_{\text{ph}}) > 0, \quad (3.4)$$

for $H > 0$, where a dot represents derivation w.r.t. the cosmological time. This counter-intuitive behaviour can also be derived purely from thermodynamic arguments [328]. At the geometric level, the accumulation of positive energy with negative pressure drives an acceleration of the universe that exceeds that produced by a cosmological constant. This phenomenon is commonly referred to as super-acceleration [329]. In non-cosmological settings, it has been also shown that phantom energy may allow for the existence of exotic geometries, such as wormholes [62, 63] (see also [45]).

Violation of the NEC is, in most cases, a sufficient condition to circumvent the classical geodesic incompleteness theorems [44, 49, 50]. Hence, singular spacetimes like those of an initial singularity or at the centre of a black hole can be made regular by invoking a phantom component [330–333]. Nevertheless, considering phantom DE may entail a different pathological behaviours. In fact, future cosmological singularities at which spacetime cease to exist typically takes place as a result from the build-up of phantom energy. However, it is important to note that this may not always be the case for phantom models [334–336], although a super-accelerated regime may have a profound impact on the structures within the universe [337].

A part from its unconventional properties, a major issue of phantom energy is the stability of the theory. This is because the violation on NEC may signal the presence of pathologies like ghosts, gradient instability and/or superluminality [69–71, 190]. In fact, the simplest realisation of an effective phantom fluid via a canonical scalar field minimally coupled to gravity faces a ghost instability

[29, 338]. NEC-violating scalar field theories with non-canonical kinetic term can avoid this problem [198, 339–342]. In the case of theories involving up-to first-order derivatives only, however, perturbations around a FLRW background solution acquired an imaginary speed of sound if they are ghost-free [160] (see also reference [1, 189, 290]). Hence, a gradient instability appears instead. Theories with higher-order derivatives may offer a promising workspace where both problems can be avoided for a phantom-like scalar field [40, 73, 198] (see also [343, 344]). Nevertheless, it is interesting to note that the introduction of higher derivatives may force the local stability properties of the scalar field to do not depend only on the scalar field variables, but also on the other matter species present locally. Indeed, this was shown to be the case of the Subluminal Galilean Genesis proposed in reference [342]. A bounce-like solution was obtained through a fully stable violation of the NEC in the absence of external matter sources. However, it was later shown that some stable solutions turn to superluminal propagation when a realistic external (subdominant) matter content was also considered [345]. A similar deceptive behaviour is also present in the late-time cosmology of the KGB theory. Ghost-free and gradient-free phantom models have been reported in, for instance, references [40, 346]. However, at least for the models discussed in [40], this apparent phantom behaviour seems to be screened by regular matter in a way that the violation of the NEC by the scalar field does not automatically lead to the violation of the NEC by the total energy-momentum tensor. In other words, even though these models feature fully stable phantom regime (where $w_\phi < -1$), the effective EOS parameter w_{eff} that governs the evolution of the geometry is greater than -1 always. It is, therefore, of great interest to raise the question of whether or not $w_{\text{eff}} + 1 \geq 0$ is a necessary condition for the interesting stability properties of the KGB theory.

Despite the fact that phantom energy is very exotic in many respects, in this thesis we advocate for an open minded approach to the presence of this type of energy in a physical theory. The reason behind this non-conservative approach is two-fold. First, it is not clear whether the violation of the NEC (either by only some component of $T_{\mu\nu}$ or at the level of the NCC) should be a no-go for any physical theory. In this regard, although this violation is usually accompanied by some instabilities in the theory, the characteristic scale at which these instabilities develop, their fate and their impact on observables must be carefully analysed before discarding the model. Second, the possibility of the expansion of the universe being fuelled by phantom-type DE is not observationally excluded [78, 79, 347]. Furthermore, it is even suggested by some data [128] and could help to alleviate the H_0 tension (see, for instance, references [129, 130]). Worthy to notice, it was also recently shown that a phantom transition is a necessary prerequisite in order to solve both H_0 and S_8 tensions simultaneously with late-time

modifications w.r.t. Λ CDM only [131, 132]. Hence, we consider that phantom models deserve an open-minded analysis as possible candidates for describing the current accelerated phase of our universe.

3.2 Classical singularities

What is a singularity of the spacetime? The idea of a singularity is intuitively connected to the divergence of the curvature of spacetime or other pathological behaviour of the metric tensor. The occurrence of these events may signal the breakdown of the classical formalism and, therefore, the loss of predictability. Besides this intuitive approach to the concept, however, a satisfactory general criterion for defining a singularity of spacetime is far from obvious. Since the curvature of spacetime is described by the Riemann tensor, $R^\mu_{\nu\theta\sigma}$, one may think of using undesirable behaviour of some of its components as a criterion for the occurrence of a singularity. However, the bad behaviour of some of its components could be simply an unfortunate product of a poorly chosen coordinate chart. Scalar quantities constructed from contractions of the Riemann tensor and/or its derivatives can evade this issue. Unfortunately, the divergence of these scalar quantities, or any polynomial built from them, may still fail to provide a general criteria for a singularity of spacetime. This is because the blow-up may occur at the infinite boundary, in which case the spacetime may not truly deserve to be dubbed as singular.

A more successful approach to the issue is that of looking for the *holes* left in your spacetime after the removal of the singularities as the very criterion for their presence (see a friendly introduction to the topic, for instance, in reference [38]). The presence of these holes should manifest through the existence of geodesics with a finite affine length, meaning they cannot be extended in (at least) one direction. These geodesics are said to be *incomplete*. The notion of incompleteness is central to classical singularity theorems, such as the Penrose-Hawking theorem [44, 348]. The proof of these theorems typically assumes the validity of some energy conditions, the absence of closed timelike curves and/or the formation of trapped regions (see reference [349] for a complete review). Additionally, singularity theorems have been discussed in the context of entropy bounds in, for instance, references [350, 351]. It is important to note, however, that singularities defined solely by geodesic incompleteness may not necessarily correspond to singularities in the curvature, and vice versa [38]. This is the case, for example, of the *parallelly propagated curvature singularity* [38, 44], where no scalar constructed from the Riemann tensor and/or its covariant derivatives blows-up, but some components of $R^\mu_{\nu\theta\sigma}$ and/or its covariant derivatives diverge when parallelly propagated along non-extendable geodesics; see also, for instance, reference [352].

Another example that illustrates the difficulty of finding a general definition for a singular spacetime is that of the *sudden* singularities [220, 221]. On a FLRW background, these are extreme acceleration events at which \ddot{a} diverge at some finite (cosmic) time, but the scale factor and its first derivative remain bounded. In view of equation (1.22), the corresponding Ricci scalar also blows-up at the sudden singularity. Nevertheless, causal geodesics have been shown to be extendable through this event [324, 353]. Thus, the sudden singularity is an example of a geodesically extendable but curvature singular model. In fact, this behaviour was also confirmed for the case of inhomogeneous and anisotropic sudden spacetimes [354].

The *strength* of a singularity is also a very subtle topic. Intuitively, a singularity may be considered to be *strong* if tidal forces are able to break the three-dimensional objects heading towards the singularity. Tipler [355] and Królak [356] proposed independently different quantifiers for this effect. These are based on the behaviour of the volume of an object, or its derivative, when reaching the singularity. Spacetime averaging has also been proposed as a measure of the strength of a singularity [357]. The evolution of bound systems within an expanding universe can also provide a qualitative idea (and a fundamental one, in the most physical sense) about the strength of a singularity [337, 358, 359]. Thus, local bound structures (e.g. Solar System, atoms, etc.) may be torn apart due to the extreme cosmological acceleration produced by some *strong* phantom models (see also [217, 360, 361]).

To circumvent the possible issues with the definition of singularity in a cosmological setting, hereon we shall consider that a boundary of spacetime is singular if either the curvature is ill-defined or geodesic incompleteness occurs [362]. Moreover, we will also make an explicit distinction between cosmic singularities that occur at finite cosmic time and abrupt events, which take place at infinite cosmic time (although bound structures are destroyed much earlier). These considerations will be exhaustive enough for the discussion of singular behaviours in homogeneous and isotropic spacetimes.

3.2.1 Metric classification of cosmic singularities

In GR there is a bijective mapping between the total energy and pressure on the left-hand side of the Friedmann and Raychaudhuri equations, and the (squared) Hubble rate and its cosmic time derivative; see equations (1.23) and (1.24). Therefore, we will refer here to the behaviour of H and \dot{H} when addressing the different cosmological events [48], rather than to the energy density and pressure as done in reference [134]. This will provide us with a kinematic classification of singularities, which depends only on the singular spacetime and not on the particular theory of

	t_s	a_s	H_s^2	$ \dot{H}_s $	Tipler	Królak
Big Bang	0	0	∞	∞	S	S
Big rip	Finite	∞	∞	∞	S	S
Big Freeze	Finite	Finite	∞	∞	W	S
Sudden	Finite	Finite	Finite	∞	W	W
Little rip	∞	∞	∞	∞	-	-
LSBR	∞	∞	∞	Finite	-	-

Table 3.1: Metric classification of the cosmic singularities/abrupt events that we will discuss here by means of the time of occurrence of the singularity t_s , and value of the scale factor a_s , the Hubble parameter H_s and its cosmic time derivative \dot{H}_s at the catastrophic event. The strength of the cosmic singularity/abrupt event is also discussed in terms of the Tipler [355] and Królak [356] criteria, where "S" stands for strong and "W" for weak.

gravity. In table 3.1 we summarise the main cosmic singularities and abrupt events that we will repeatedly discuss in this manuscript. Please note that, singularities corresponding to contracting cosmologies (e.g. the big crunch [362]) will not be addressed here since we focus on the DE phenomenology assuming that this component is repulsive today and will remain so in the future. For the same reason, turnaround and/or bounce-like events will also be omitted from the discussion. The reader further interested in the general behaviour, both at the kinematical and dynamical level, of cosmological milestones may also find interesting the reference [363] (see also [353, 364]). Different nomenclatures for the classification of singularities in GR may be found references [365–367], and references [368–370] for modified theories of gravity.

Big Bang (BB) This is an initial singularity (i.e. it takes place at $t_s = 0$) where the scale factor vanishes, but the Hubble rate and its cosmic time derivative diverge [362]. Causal geodesics are past incomplete [371]. Please note that this is not a DE-induced singularity. In fact, the standard version of the hot big bang model corresponds to an adiabatically expanding radiation-dominated FLRW universe [362]. This cosmic singularity is catalogued as TYPE I.A in reference [48], whereas in reference [367] it is labelled as TYPE 0. According to the criteria of Tipler [355] and Królak [356], this is a strong singularity where the volume characterizing a three-dimensional object and its proper-time derivative, respectively, are crashed to zero when propagated backwards (in time) along causal geodesics.

Big Rip (BR) This is a future singularity at which the size of the observable universe along with the Hubble rate and its cosmic time derivative diverge. It

takes place at a finite cosmic time, t_s , since the integral

$$\int_{t_0}^{t_s} dt = \int_{a_0}^{\infty} \frac{da}{aH(a)}, \quad (3.5)$$

converges. The BR is intrinsic to DE models with phantom behaviour [88, 217] (see also [59, 61, 290, 372, 373]). Time-like geodesics describing free-falling observers are future incomplete [353]. They reach a curvature singularity in a finite proper time. However, null geodesics are complete for a constant EOS parameter, w , near the BR in the range of $-5/3 < w < -1$ [353]. That is, photons only experience the BR singularity if $w < -5/3$ [353]. This limiting value for w was dubbed as super-phantom in reference [61] for the case of a flat FLRW background with a constant EOS parameter. In the nomenclature of both references [134] (see also [48]) and [367], this phantom-DE cosmic singularity is catalogued as TYPE I. Moreover, the BR singularity is the only DE-induced (future) cosmic singularity that is strong according to both Tipler [355] and Królak [356] criteria. In reference [364], it was shown that a BR-like fate is also possible for models with an EOS parameter that converges to -1 from the phantom zone. For these models, the divergence of the scale factor, the Hubble rate and its cosmic time derivative was shown to be faster than in the standard BR picture [364]. Owing to this reason, they were dubbed as grand rip [364] and classified as TYPE -1 singularities [374]. (See also reference [4] for other examples of grand rips.) For this doomsday, time-like geodesics are incomplete and, therefore, all inertial observers meet the curvature singularity in finite proper time [364]. Nevertheless, null geodesics avoid reaching the singularity and are complete in that direction [364], which is similar to what happens in the *standard* non-super-phantom BR scenario [353]. Moreover, the grand rip is also a strong curvature singularity according to Tipler [355] and Królak [356] criteria. Since both the BR and grand rip have qualitatively the same behaviour in terms of the time of occurrence (finite), the size of the observable universe (infinite), and the value of the Hubble rate (infinite) and its time derivative (infinite) evaluated on approaching the singularity, hereon we will not address the possible differences between these events. Hence, we keep the term *big rip* for both of them.

Big Freeze (BF) This is a curvature singularity that occurs at a finite cosmic time with a finite value for the scale factor, but at which the Hubble rate and its cosmic time derivative diverge [218, 219] (see also [133, 135, 375]). Due to the finite value of the scale factor at the BF, this singularity belongs to the so-called group of *finite scale factor* singularities [367] (see also [376]). In both references [134] (see also [48]) and [367], this is labelled as TYPE III event. The BF appears, for example, for the EOS given by $p = -\rho - \mathcal{A}\rho^\alpha$ [135], when \mathcal{A} is positive and $\alpha > 1$ (see also table 2 in reference [4]). It was also discussed in the generalised Chaplygin gas $p = -\mathcal{A}/\rho^\alpha$ [219]. Since the scale factor converges to a finite value,

causal geodesic reach the BF singularity within finite affine parameter. Moreover, the velocities along causal geodesics are finite [377], but the acceleration diverge. Accordingly, the geodesic equations are not well-defined at the singularity and, therefore, no extension through the BF is possible. Thus, causal geodesics are incomplete. The Tipler [355] and Królak [356] criteria do not give the same result for the strength of the BF. According to the former, this is a weak event. However, it is a strong singularity from the point of view of the latter. Bound structures are not necessarily destroyed at the BF singularity [361].

Sudden This occurs at a finite scale factor, the Hubble rate is also finite but its cosmic time derivative diverge [220, 221]. Moreover, the sudden singularity takes place at a finite cosmic time t . In references [134, 367] (see also [48]) this singularity is labelled as TYPE II. It has also been referred to as sudden past/future singularity depending whether it takes place in the past or future evolution of the system [220]. In GR, the sudden singularity represents an extreme pressure event, which provokes the blow-up of the acceleration, \ddot{a} , to plus/minus infinity. Causal geodesics reach the sudden singularity in a finite proper length. However, geodesic can be extended through this event and only the equations for geodesic deviation remain singular [324, 353]. Hence, point-like particles travelling along causal geodesics do not even see the sudden singularity, while extended objects may suffer instantaneous infinite tidal forces [324, 378]. According to both Tipler [355] and Królak [356], the sudden is a weak cosmic singularity. Consequently, tidal forces are not strong enough to crush to zero all finite bodies. As mentioned before, the sudden singularity is an example of a geodesically complete but curvature singular model. This behaviour was also confirmed for the case of inhomogeneous and anisotropic sudden spacetimes [354]. Note that some particular cases of the sudden scenario have been given special names in the literature. This is the case of the *big brake* singularity [379, 380] (see also [298, 381]), at which the expansion of the universe comes into an abrupt halt in the future due to an extreme deceleration. Conversely, the universe may have experienced an extremely large acceleration in the past due to a very negative pressure at a *big démarrage* singularity [299]. The occurrence of the big brake and big démarrage can be found in, for example, a universe filled with a perfect fluid obeying the generalized Chaplygin gas characterised by $p = -\mathcal{A}/\rho^\alpha$ [219]. See also references [378, 382, 383] for further discussion on sudden models.

The cosmic events mentioned above do not constitute an exhaustive list of all possible cosmological singularities. Just to briefly mention some other pathological behaviours, there are cosmological models for which the Hubble rate and its first derivative are well-defined, but higher order derivatives diverge for a finite value of the scale factor and within a finite cosmic time. This is the case of the generalised

sudden singularities [221] (see also TYPE IV in references [48, 375] and TYPE II_g in reference [367]). Another possibility is having a vanishing Hubble rate at a finite scale factor, whereas its cosmic time derivative remains finite in such a way that the EOS parameter, w , diverge. This is the so-called w -singularity [384] (see also [385]) and it may have effects in the linear order cosmological perturbations. A third, but not last, scenario is that of the interacting DE-DM models in which the interacting term Q blows-up at finite cosmic time [377]. While the occurrence of a Q -singularity does not imply any pathological behaviour at the background level, it might lead to the divergence of the speed of sound related to the perturbations. However, we will not explore here any further these or other possible singular events in cosmology. We refer the interested reader to the reviews [386, 387], and references therein.

3.2.2 Abrupt events

Previously, we have referred to cosmological singularities as those catastrophic events that take place at a finite cosmic time t_s . We will now discuss the occurrence of abrupt events in cosmology, where this term refers to a cosmological curvature singularity that takes place at infinite cosmic time but for which bound structures may be destroyed in the near future.

Little Rip (LR) This abrupt event can be understood as a BR singularity that has been postponed indefinitely. At the LR, the scale factor, the Hubble rate and its cosmic time derivative explode in the infinite asymptotic future [388]. This infinitely-late BR appears in phantom DE models with a w -parameter rapidly converging to the cosmological constant value ($w = -1$) so that the occurrence of a future *rip* is delayed indefinitely in time [135, 389] (see also [388, 390]). Even though the divergence formally occurs at $t_s \rightarrow \infty$, bound structures are shown to be disintegrated at a finite time from present [388]. The name “little rip” was originally coined for the DE model with an EOS given by $p = -\rho - \mathcal{A}\sqrt{\rho}$, where \mathcal{A} is a positive constant, in reference [388]. Nevertheless, this cosmological behaviour was already known from before for that EOS [135]. In fact, see also [389] where a fate *à la* LR was found in brane cosmology and before that in some modified theories of gravity [391].

Little Sibling of the Big Rip (LSBR) In this scenario, the size of the observable universe and the expansion rate grow infinitely big, but the cosmic time derivative of the Hubble parameter converges to a constant value [360]. The EOS parameter for the DE component behaves similarly as in the LR case: it quickly converges to -1 from the phantom region [360]. Nevertheless, bound structures in the universe are destroyed in a finite cosmic time from now [360]. This abrupt

event was first noticed for the DE model with an EOS given by $p = -\rho - \mathcal{A}$ [360], with \mathcal{A} a positive constant.

Please note that the definition of an abrupt event as a curvature singularity excludes the interesting case of the pseudo-rip from the above discussion [335] (see also reference [334] for early phantom models featuring this behaviour). This is a *mild* event at which the Hubble parameter becomes an increasing function on time that converges to a constant value. The corresponding curvature is always non-singular and the asymptotic future state is effectively that of a dS [334, 335]. Nevertheless, the dS solution is approached from the phantom zone. That is, \dot{H} is positive before reaching the dS regime, contrary to the Λ CDM case where $\dot{H} \leq 0$ always. Hence, these models have been considered as an intermediate case between the LR and the cosmological constant [335]. However, finite-time disintegration of bound structures may occur due to the phantom nature of these models [335] (see also [336]).

3.3 Quantum cosmology

Spacetime singularities appear to be an inevitable prediction of GR [348]. From the initial BB singularity, to the formation of black holes and the occurrence of future catastrophic events in (not only) phantom cosmology. Nevertheless, it is commonly believed that a complete and consistent quantum description of the universe may prevent the appearance of classical singularities, see references [297, 298] (see also [48, 133, 134, 299, 392, 393]). Even though there is a lack of consensus on what is the correct quantum theory of gravity, the application of ordinary quantum mechanics to the universe as a whole leads to an interesting framework for addressing the issue of classical singularities. This is known as quantum cosmology (for a review of the topic see, e.g., references [394, 395]). Currently there are multiple proposals to quantize the cosmological background. A non-exhaustive listing of different approaches to quantum cosmology is string theory (see, for instance, the review [396]), causal dynamical triangulation [397–399] and canonical quantizations of GR [400–402], among other examples (see also reference [394]). Nonetheless, in this thesis we shall focus only on the latter approach, which corresponds, in fact, to one of the earliest attempts to quantize cosmological backgrounds [400]. Hence, in this section we briefly introduce some features of the different canonical approaches to quantum cosmology, focusing on the relevant framework that will be employed later in chapter 6.

At the core of any canonical quantization lies the Hamiltonian formulation of GR. Using a (3+1)-decomposition of spacetime it is possible to define a Hamiltonian at each spatial hypersurface [403]. In GR, there are four local (secondary)

constraints that cover the entire dynamics of the theory and are completely equivalent to the Einstein's equations. These are the Hamiltonian and momentum (diffeomorphism) constraints expressed as

$$\mathcal{H}_0 = 0 \quad \text{and} \quad \mathcal{H}_i = 0, \quad (3.6)$$

respectively. Up-to boundary terms, the total Hamiltonian reads

$$\mathcal{H} = \int d^3x (N\mathcal{H}_0 + N^i\mathcal{H}_i), \quad (3.7)$$

being N and N^i the lapse and shift functions, respectively, which act as Lagrange multipliers in GR (see, for instance, reference [404] for modified theories of gravity). This is the starting point of the canonical quantization approach to quantum gravity. Now, the canonical variables on which to perform a certain quantization scheme should be selected. It is at this point where different canonical quantum theories first branch-out.

3.3.1 Quantum geometrodynamics

The more straightforward (and conservative) approach would be to select the induced spatial-metric h_{ij} and its conjugate momenta p^{ij} , related to the extrinsic curvature, as the configuration variables [394, 400]. Up-on quantization, these variables are promoted to operators according to

$$\hat{h}_{ab}\Psi[h_{cd}] = h_{ab}\Psi[h_{cd}], \quad (3.8)$$

$$\hat{p}^{ab}\Psi[h_{cd}] = -i\hbar\frac{\delta\Psi[h_{cd}]}{\delta h_{ab}}, \quad (3.9)$$

being Ψ the wave function describing the quantum state of the system, which is also known as the *wave function of the universe* [400] (see also reference [405] for arguments in defence of this picture). This wave function depends on the induced metric h_{cd} and the non-gravitational external fields to the Einstein-Hilbert action (when considered). This quantization procedure leads to the theory of quantum geometrodynamics and represents, in fact, the oldest approach to quantum gravity [400, 406] (see also [407]). The first minisuperspace model in quantum cosmology was also presented in DeWitt's pioneering work [400]. Here, the expression minisuperspace is derived from the nomenclature of *superspace* to denote the (infinite) space of all three-dimensional metrics h_{ab} (and all matter field configurations). The prefix *mini* is added to indicate the truncation of this space to a finite number of DOFs corresponding to the cosmological background.

In homogeneous backgrounds, the Hamiltonian constraint contains all the dynamical information at the classical level, since the momentum constraint is satisfied automatically. In quantum geometrodynamics, the canonical quantization of

the \mathcal{H}_0 constraint leads to the Wheeler-DeWitt (WDW) equation [400, 406]. This functional differential equation plays a central role in quantum geometrodynamics comparable to that of the Schrödinger in quantum mechanics. Schematically, it reads [400, 406]

$$\hat{\mathcal{H}}_0 \Psi [h_{ab}] = 0, \quad (3.10)$$

where \mathcal{H}_0 has been promoted to operator acting on Ψ according to the above quantization scheme. In chapter 6 we will address in details the structure of \mathcal{H}_0 and its quantization to $\hat{\mathcal{H}}_0$ in the case of $f(R)$ theories of gravity. For introductory purposes, nevertheless, general features of this equation can be highlighted using its conventional expression in GR. In the absence of non-gravitational DOF, this equation takes the form [394, 400]

$$\left(-2\hbar^2 G_{ijkl} \frac{\delta^2}{\delta h_{ij} \delta h_{kl}} - \frac{\sqrt{\hbar}}{2} \left({}^{(3)}R - 2\Lambda \right) \right) \Psi [h_{ab}] = 0, \quad (3.11)$$

where G_{ijkl} is called the DeWitt metric. First of all, note that the WDW equation is a (functional) equation defined in configuration space. It does not depend on spacetime points, as may be expected from the quantization of a diffeomorphism-invariant theory [395]. Second, there is not an external time parameter: the WDW equation is timeless. This may sound somehow obvious since there appear no coordinates. However, neither there is a unique way to define an internal time-like variable in the minisuperspace [395]. This is known as *the problem of time* and is also present in other attempts towards a quantum theory of gravity [408, 409]. Luckily, the WDW equation is locally hyperbolic under certain circumstances [400], which opens a window to the possibility of identifying a configuration space variable as an internal time-like parameter from the very wave-like structure of the equation¹ [408, 409, 411]. The hyperbolic signature, however, is not a general feature of the WDW equation. If a canonical minimally coupled phantom scalar field is also considered, then, the resulting WDW equation becomes elliptic or ultrahyperbolic [297]. Moreover, it was also shown that the signature can become elliptic in some regions of the configuration space for a FLRW minisuperspace model with a non-minimally coupled scalar field [412]. In third place, we shall also mention the *factor-ordering* problem related to the kinetic term in expression (3.11). This is the open issue of whether or not additional terms proportional to \hbar containing at most first (functional) derivatives of the metric should also appear [394]. Lastly, we shall emphasize that quantum geometrodynamics is a non-perturbative attempt to quantize gravity. Moreover, even if it is replaced at the Planck scale by a more fundamental quantum theory of gravity, it is argued that this should be the right semi-classical limit connecting with GR [411].

¹In FLRW this is usually the scale factor or $\ln a$ [410] (see also [297, 395, 409]).

DeWitt also proposed a boundary condition for the avoidance of classical singularities within the quantum regime [400], namely the DeWitt (DW) criterion. According to this, classical singularities are (potentially) avoided if the wave function vanishes at the singular configurations in the minisuperspace. That is [400]

$$\Psi \left[h_{ab}^{(s)} \right] = 0, \quad (3.12)$$

where $h_{ab}^{(s)}$ is the singular induced metric. Recall that we only consider gravitational DOFs here for the sake of the introduction. If non-gravitational DOFs are added, e.g. a scalar field ϕ , the dimension of the minisuperspace is augmented by the corresponding terms. The DW criterion can be understood as a generalization of the interpretation usually given to the wave function in ordinary quantum theory, where the wave function is the fundamental building block for any observable. Consequently, regions of the configuration space that lay outside of the support of Ψ are, therefore, *irrelevant* for the classical physicist. Alternatively to this interpretation, the wave function Ψ can be linked in a heuristic way with the probability distribution [413]. In that sense, having a vanishing wave function could be interpreted as having zero probability of reaching that point in the configuration space [400]. Nevertheless, this interpretation is based on the existence of squared integral functions and a consistent probability interpretation of the wave function. The problem is, however, that these assumptions would require a minisuperspace with a proper Hilbert structure, and that is not obvious to be always doable (or even necessary [395]) for a quantum cosmology based on the WDW equation [394] (see also the review [386]). Anyway, it should be noted that the non-vanishing of the wave function does not necessary entail a singularity [48]. Therefore, the DW criterion can only be a sufficient but not necessary criterion for the avoidance of classical singularities in the quantum regime. See references [48, 395, 411] for a friendly introduction to the topic.

The DW criterion has been successfully applied in the context of several cosmological singularities in FLRW like, for instance, the BB [297, 414], the BF [299], the BR [414], the LR [304], the LSBR [302] and some particular cases of sudden singularities [298, 299] (see also reference [48] for a review). The DW criterion has also been discussed for the BR singularity in the context of Bianchi I cosmology [415] and Eddington-inspired-Born-Infeld theory [414, 416–418]. Singularity avoidance for collapsing dust clouds has been addressed in, for instance, references [419–421]. In the framework of metric $f(R)$ theories of gravity, see also the avoidance of the BR [422], the LR [5] and the LSBR [6], where further comments may be found in reference [4].

Alternatively to the DW criterion, the dispersion of wave-packet solutions to the Wheeler–DeWitt equation when approaching the classical singularity has also been considered as indicative for singularity avoidance [297]. In this approach,

the dispersion of the wave-packets signals the breakdown of the semi-classical approximation and, therefore, the very concepts of time and classical evolution cease to exist before reaching the classical singularity. In this interpretation, the classical evolution becomes singularity-free [297] (see also [48, 394]).

3.3.2 Loop quantum cosmology

For the sake of completeness, we shall briefly mention the other main canonical quantization approach to quantum cosmology: loop quantum cosmology [401, 423]. Quantum geometrodynamics and loop quantum cosmology first branch-out in the choice of the dynamical variables before quantization. Whereas in the former case we select the spatial metric and its conjugate momenta, in *loops* the Ashtekar's variables are used instead [401, 423]. These are related to a $SU(2)$ connection and a triad density. On FLRW, they are parametrized by a new pair of canonical variables, $c(t)$ and $p(t)$, related to the scale factor and its cosmic time derivative, respectively [394].

The singularity avoidance in loop quantum cosmology can be addressed by noting that different physical quantities that diverge (or vanishes) at the classical singularity have now bounded (or different from zero) expectation values [424]. Singularity avoidance is also often discussed not at the level of expectation values but in terms of the effective modifications to the Einstein equations [425] (see also [426]). In fact, the (total) energy density appearing in the Friedmann equation (1.23) is modified as [425]

$$\varrho \longrightarrow \varrho \left(1 - \frac{\varrho}{\varrho_{\text{crit}}} \right), \quad (3.13)$$

begin ϱ_{crit} a critical density inversely proportional to the smallest non-zero eigenvalue of the area operator [424, 425]. This correction sets an upper bound to the possible value of the classical energy density in the theory, at which the observable universe reaches maximum/minimum size. In this way, the initial BB singularity ($\varrho \rightarrow \infty$ as $a \rightarrow 0$) is replaced with a big bounce connecting a contracting and an expanding branch at the critical scale [427–429]. Similar conclusions have also been reached for phantom-induced future BR and BF singularities [430, 431]. Thus, these classical doomsdays are replaced with a transition to a recollapsing branch of the universe at the critical scale [430, 431]. Away from this critical value, however, the effective modification to the Friedmann equation becomes negligible.

Part II

Kinetic gravity braiding theory

4 Shift-symmetric scalar field theory

SCALAR FIELD theories could be crucial in providing an underlying theoretical framework for addressing the mysteries of DE. These theories introduce a scalar field that can be used to describe dynamical DE component, in contrast to the cosmological constant case (see, for instance, references [26, 29, 115]). Among the different scalar field theories introduced in section 2.2, the KGB framework has already proven to be extremely fruitful in both early- and late-time cosmology; see, for instance, applications to inflation in references [96, 158, 196–198] and DE models [40, 168, 189, 199–207]. The KGB models are a subclass of the more general Horndeski theory [99] (see also reference [155] for a review), and, therefore, they have second-order field equations. Furthermore, the KGB model trivially allows gravitational waves to propagate at the speed of light [99], which is in agreement with the recent observation of the GW170817 event [165]. In addition, the parameter space of the theory has also been confronted with cosmological observables [208–212], rendering this set-up as a viable DE candidate. Nevertheless, note that some specific KGB models may be found at tension with cosmological data (see, for example, the discussion on Cubic Galilean gravity in references [213–215]). The KGB set-up has also been studied in the context of the H_0 tension, showing a possible modest increase in the value of H_0 [175]. Moreover, the Palatini version of the KGB theory and its connection to the metric formalism have been previously explored in reference [216].

As previously discussed, one of the arguments most commonly used to go beyond the standard model of cosmology is the existence of a fine-tuning problem regarding the value of the cosmological constant [24, 25]. A general problem of scalar theories, however, is that having potential-like terms could reintroduce the fine-tuning problem now regarding the parameters that fix the minimum of the potential at the equilibrium point, if the accelerated expansion is reached in the potential domination regime. One possible way of trying to avoid this problem is the consideration of a shift-symmetric scalar field, which guarantees that the cosmic acceleration is driven by the kinetic energy [201, 265]. We recall that shift-symmetry makes the action of the theory invariant under constant shifts in the scalar field, i.e

$$\phi \rightarrow \phi + c, \tag{4.1}$$

being c a constant. However, the simplest minimally coupled scalar field with

a canonical kinetic term in the action is only able to describe a stiff fluid when imposing shift-symmetry (see, for example, references [29, 95]); leading to a non-interesting phenomenology for the (late-time) DE sector. When this symmetry is imposed on the viable Horndeski family (2.12), it reduces the parameter space to that of the shift-symmetric KGB theory only. Hence, $f(R)$ theories of gravity in their scalar field representation are ruled-out by this symmetry argument.

The shift-symmetric KGB models are well-known for the possibility of driving the expansion of the cosmos towards a future self-tuning dS (dS) state [40]. Consequently, they have naturally attracted considerable attention (see, for instance, references [168, 199–203, 207]). In addition, the effective DE component obtained in this fashion can exhibit phantom behaviour that is stable at first order in perturbation theory [40], i.e. free from ghost and gradient instabilities. We remind the reader that phantom DE is characterized by an EOS parameter w_{DE} less than -1. This is a real possibility that is not only observationally feasible [78, 79, 347], but was analytically shown to be a prerequisite for alleviating both the H_0 and σ_8 tensions simultaneously by means of late-time modifications to Λ CDM only [131, 132]. Therefore, the motivation, simplicity and apparent stability properties of the shift-symmetric KGB scalar field models makes this framework an interesting proposal for modelling DE.

Nevertheless, it is a general property of phantom DE that the evolution of the universe could entail a future cosmological singularity or abrupt event. Examples of such scenarios include a future BF, BR, LR, or LSBR events, which are indeed intrinsic to phantom cosmologies. Therefore, since the future phenomenology of phantom DE models could encompass a broad variety of singular behaviours, it is natural to wonder whether the (stable phantom) DE component modelled in the shift-symmetric KGB theories could lead the evolution of the cosmos towards a different future state from that of the well-studied dS future solution of the theory. In other words, the question arises whether a future dS is the only possible attractor in the configuration space of the shift-symmetric KGB framework.

In this chapter we address the latter question. By reviewing the assumptions underlying the existence of these future dS attractors we argue for the possibility of different future evolutions for the system. In order to support these claims, we propose a dynamical system formulation for the KGB theory different from the previously used in the literature (see, for example, references [168, 199, 201, 203, 207]). Within this new approach, we study the fixed points of the system and the stability of the orbits in the configuration space.

This chapter is based on the peer-reviewed publications [2, 3]. The discussion is organized as follows: section 4.1 provides an introduction to the shift-symmetric KGB theories and their application to a homogenous and isotropic cosmological background. Section 4.2 is devoted to the dynamical system formulation of an

expanding universe in the shift-symmetric KGB set-up. Moreover, different power law KGB models are analysed in sections 4.3 and 4.4. Lastly, concluding remarks shall be found in section 5.3. Appendices A and B contain clarification notes.

4.1 Shift-symmetric kinetic gravity braiding theories

The shift-symmetric KGB theory follows from demanding the general KGB action (2.21) to be invariant under constant shifts in the scalar field. This produces [40]

$$S = \int d^4x \sqrt{-g} \left[\frac{1}{2}R + K(X) - G(X)\square\phi \right], \quad (4.2)$$

where we recall that we have adopted the geometric unit system $8\pi G = c = 1$. Contrary to the full KGB theory (2.21), the functions K and G now depend only on kinetic term $X := -\frac{1}{2}g^{\mu\nu}\nabla_\mu\phi\nabla_\nu\phi$ due to the shift-symmetry [40]. In fact, the shift-symmetric KGB theory represents the only non-trivial shift-symmetric theory in the viable Horndeski (2.12) up-on constant redefinitions of the gravity coupling constant.

For a cosmological background described by the homogeneous and isotropic spatially flat FLRW spacetime (1.21), the Friedmann and Raychaudhuri equations read [40]

$$3H^2 = \varrho_m + \varrho_r - K + \dot{\phi}J, \quad (4.3)$$

$$\dot{H} = -\frac{1}{2} \left(\varrho_m + \frac{4}{3}\varrho_r \right) + XG_X\ddot{\phi} - \frac{1}{2}\dot{\phi}J, \quad (4.4)$$

where we have assumed matter and radiation as external sources to the action (4.2), a dot represents derivation w.r.t. the cosmic time t and G_X stands for dG/dX . The conservation of these external sources run as usual,

$$\dot{\varrho}_m = -3H\varrho_m, \quad (4.5)$$

$$\dot{\varrho}_r = -4H\varrho_r, \quad (4.6)$$

being ϱ_r and ϱ_m the energy densities for radiation and matter, respectively. In addition,

$$J(\dot{\phi}, H) := \dot{\phi}K_X + 6HXG_X, \quad (4.7)$$

is the shift-current related to the global shift-symmetry of the theory [40]. On the flat FLRW spacetime, the general energy density (2.23) and pressure (2.24) of the dark fluid reduce to

$$\varrho_\phi(\dot{\phi}, H) := \dot{\phi}J - K, \quad (4.8)$$

and

$$p_\phi(\dot{\phi}, \ddot{\phi}) := K - 2XG_X\ddot{\phi}, \quad (4.9)$$

respectively. Contrary to k -essence [96], please note that the energy density, ϱ_ϕ , now depends on the Hubble parameter through J while the pressure, p_ϕ , contains $\ddot{\phi}$ [40]. Moreover, the pressure will also show an explicit dependence on the Hubble function (and the external sources) when $\ddot{\phi}$ is removed using the field equations; see appendix A. Also note that the flux vector q^μ computed in expression (2.30) is trivial on FLRW. As commented in section 4.1, this means that the background evolution on FLRW can be equivalently described with a perfect fluid approximation for the scalar field. For general backgrounds, however, the fluid will be *imperfect* due to non-trivial energy flow [41].

The field equation of the scalar field can be obtained varying the action (2.21) w.r.t. the scalar field. This yields

$$A(\dot{\phi}, H)\ddot{\phi} + 6XG_X\dot{H} + 3HJ = 0, \quad (4.10)$$

where

$$A(\dot{\phi}, H) := K_X + 2XK_{XX} + 6H\dot{\phi}(G_X + XG_{XX}), \quad (4.11)$$

has been defined for the compactness of the notation. It is indeed easy to show that this equation is completely equivalent to the covariant conservation of the ϕ -fluid in the hydrodynamic approach, that is

$$\dot{\varrho}_\phi + 3H(\varrho_\phi + p_\phi) = 0, \quad (4.12)$$

where ϱ_ϕ and p_ϕ correspond to the scalar field energy density and pressure defined in expressions (4.8) and (4.9), respectively. It should be noted, however, that the scalar field equation of motion (either in the form of equation (4.10) or, equivalently, in the hydrodynamic approach depicted in equation (4.12)) is not independent from the system of equations given in expressions (4.3) to (4.6).

Alternatively to the scalar field equation (4.10), one can obtain the same information from the conservation equation related to the shift-symmetry of the theory; that is

$$\frac{1}{a^3} \frac{d(a^3 J)}{dt} = 0. \quad (4.13)$$

As noted in the reference [40], this conservation trivially leads to a first integral of motion for the system given by

$$J = Q_0 \left(\frac{a}{a_0} \right)^{-3}, \quad (4.14)$$

where Q_0 is a constant and a_0 the current value of the scale factor. Equation (4.14) implies that J is either trivial, that is if and only if $Q_0 \equiv 0$, or vanishes asymptotically for infinitely expanding FLRW universe. Hence, the vanishing of this shift-current can be used to extract information about the future evolution of the theory [40]. It should be mentioned, however, that $J = 0$ does not represent a proper fixed point of the system but a surface in the corresponding configuration space. This is because equations (4.3), (4.4), (4.5), (4.6) and (4.13) define a three-dimensional configuration space, as they consist of four dynamical equations along with one constraint equation. Consequently, the condition $J = 0$ defines a surface in that configuration space. Moreover, this surface either contains all the trajectories in the configuration space, if $Q_0 = 0$, or it will be asymptotically intersected by the evolution of the system if the scale factor diverges.

Let us reflect a bit more on this crucial point. In the case of a trivial shift-charge, no explicit scale factor dependence is present in the shift-current (4.14). Consequently, the Friedmann (4.3) and Raychaudhuri (4.4) equations simplify as the term $\dot{\phi}J$ drops out. Then, the evolution of the system could tend to a (quasi)dS state provided that the k-essence function K converges asymptotically to a negative constant and the slow-roll condition $XG_X\ddot{\phi} \approx 0$ is satisfied. The presence of a dS future attractor in the shift-symmetric KGB models was first discussed in reference [40] and has indeed gathered considerable attention ever since; see, for instance, references [168, 199–203, 207]. (These trajectories within the configuration space that lead to a future dS state are sometimes dubbed *tracker* trajectories [201, 207].) Conversely, if $Q_0 \neq 0$, the shift-current is not exactly zero but scales with the expansion. As a result, this scenario may present a broader phenomenology than in the previous case. In fact, if the scalar field velocity increases faster than a^3 with the expansion, then the contribution of $\dot{\phi}J$ to the total energy and pressure diverge. This could lead the evolution of the model towards a very different future fate from that of an asymptotic dS state. Note that, the energy density and pressure of the scalar field may actually diverge if $\dot{\phi}J$ blows-up; see equations (4.8) and (4.9). Therefore, the future evolution in that case could entail a BR singularity provided that the divergence takes place at a finite cosmic time [2]. The future phenomenology for a non-trivial shift-charge was also explored in references [216, 432, 433].

4.2 Dynamical system analysis

The existence of future cosmological singularities in the shift-symmetric KGB theory is properly addressed in this section with a dynamical-systems formulation. This allows for a systematic study of the fixed points of the theory and their stability. To this end, it is important to note that equations (4.3), (4.4), (4.5), (4.6)

and (4.13) are not all independent from each other. This is because they represent four dynamical equations and one constraint. As a result, a three-dimensional configuration space is to be expected.

4.2.1 The autonomous system

In view of the Friedmann equation (4.3), we proceed as usual and define the dimensionless variables

$$\Omega_r := \frac{\varrho_r}{3H^2}, \quad (4.15)$$

$$\Omega_m := \frac{\varrho_m}{3H^2}, \quad (4.16)$$

$$\Omega_\phi := \frac{\epsilon\sqrt{2X}J - K}{3H^2}, \quad (4.17)$$

where $\epsilon := \text{sgn } \dot{\phi}$ labels the increasing and decreasing branches for the scalar field. Moreover, we assume Ω_ϕ to be positive since we are mainly interested in the future attractors of expanding FLRW models. Hence, $\Omega_i \in [0, 1]$ for $i \in \{r, m, \phi\}$. In terms of these variables, the Friedmann equation (4.3) can be expressed as

$$\Omega_r + \Omega_m + \Omega_\phi = 1. \quad (4.18)$$

This is a constraint equation rather than a dynamical one. Hence, this relation can be used to eliminate one of the aforementioned variables from the system. We select Ω_m as the variable to be eliminated. Then, a new independent variable should be introduced in order to obtain the three-dimensional autonomous system. We select this new variable, h , as the following compactification scheme for the Hubble rate [277]

$$\frac{H}{H_0} = \frac{h}{1 - h^2}, \quad (4.19)$$

being H_0 the current value of the Hubble parameter. Note that this transformation represents a bijective mapping of the H -line onto the compact segment¹ $[-1, 1]$. However, since we are not interested in contracting FLRW models ($H < 0$), we shall restrict to $h \in [0, 1]$. It should be emphasized that compact variables are highly recommended, otherwise fixed points at the infinite boundary of the system

¹This compactification is similar to the *arctan* (or *arctanh*) prescription. However, the polynomial compactification (4.19) was argued to be more convenient for the proper identification and classification of the fixed points, if any, at H -infinity; see reference [277] and references therein.

may be overlooked. In terms of these new variables the evolution of the system given by equations (4.4), (4.6) and (4.13) reads

$$h' = \frac{(1 - h^2)h}{1 + h^2} C_1, \quad (4.20)$$

$$\Omega_r' = -2\Omega_r(2 + C_1), \quad (4.21)$$

$$\Omega_\phi' = C_2 - 2\Omega_\phi C_1, \quad (4.22)$$

with the auxiliary functions

$$C_1 := \frac{H'}{H}, \quad (4.23)$$

$$C_2 := \frac{\epsilon\sqrt{2X}}{H^2} (HG_X X' - J), \quad (4.24)$$

which, in general, depend on the variables h , Ω_ϕ and Ω_r since H' and X' can be re-expressed in terms of these variables; please find the details in appendix A. Also mind that Ω_m has been eliminated from the dynamical system by means of the Friedmann constraint (4.18). The prime in the above expressions denotes differentiation with respect to the dimensionless time-like variable

$$\lambda := \ln(a/a_0), \quad (4.25)$$

from which it follows that

$$\frac{d}{d\lambda}(\cdot) = H^{-1} \frac{d}{dt}(\cdot), \quad (4.26)$$

being t the cosmological time. It should be emphasised, however, that this definition for the independent variable, λ , of the system is only well-defined for monotonically expanding geometries. Therefore, recollapsing (turnaround) cosmologies or bounce-like events are excluded from our analysis. In fact, the dynamical variables (4.15)-(4.17) are not even well-suited for addressing the existence of fixed points corresponding to these events. Since a bounce/turnaround would take place at a finite scale factor with vanishing Hubble rate the partial densities (4.15)-(4.17) we have selected as the dynamical variables would diverge. Recollapsing cosmologies and bounce solutions in KGB theories have been previously addressed, for instance, in reference [216]. Equilibrium points corresponding to purely contracting FLRW models are also excluded from our discussion. Nevertheless, it should be pointed out that each fixed point for the expanding geometry would have an exact counterpart in a contracting universe due to the symmetry of the background equations under inversion of time. The stability in the contracting regime would be the opposite to that of the expanding case since reversing the time (i.e. $\lambda \rightarrow -\lambda$) also reverses the flow defined by (4.20)-(4.22) and, therefore,

the stability of the equilibrium points. The interested reader may find further information on dynamical systems and their applications to cosmology in references [269, 270, 274, 275, 278, 280].

The auxiliary functions C_1 and C_2 can be seen as functions on the new variables defined in (4.15), (4.17) and (4.19). That is $C_i(h, \Omega_\phi, \Omega_r)$ for $i \in \{1, 2\}$. These functions are connected with the effective EOS parameter of the total fluid and the EOS parameter of the scalar field contribution. The former is

$$w_{\text{eff}} := \frac{P_{\text{tot}}}{\rho_{\text{tot}}} = -1 - \frac{2}{3}C_1. \quad (4.27)$$

Whereas for the latter, one can directly read from the energy density (4.8) and pressure (4.9) that

$$w_\phi := \frac{p_\phi}{\rho_\phi} = -1 - \frac{1}{3\Omega_\phi}C_2. \quad (4.28)$$

Hence, the auxiliary functions C_1 and C_2 , which play a crucial role in realizing a closed dynamical system, are also physically significant for characterizing the system's fixed points.

4.2.2 Classification of the fixed points

Owing to the general structure of the dynamical equations (4.20)-(4.22), the fixed points $(h^{\text{fp}}, \Omega_\phi^{\text{fp}}, \Omega_r^{\text{fp}})$ of the system can be divided into five different groups², where the superscript “fp” denotes the value of the corresponding quantity at the fixed point. These groups are defined as follows, where C_i^{fp} should be read as $C_i(h^{\text{fp}}, \Omega_\phi^{\text{fp}}, \Omega_r^{\text{fp}})$:

Group 1 ($h^{\text{fp}} = \Omega_r^{\text{fp}} = 0$, $C_1^{\text{fp}} \neq -2$ and $C_2^{\text{fp}} = 2C_1^{\text{fp}}\Omega_\phi^{\text{fp}}$): Vacuum solutions. The evolution of the system in the neighbourhood of these fixed points is either dominated by matter or the scalar field.

Group 2 ($h^{\text{fp}} = 0$, $C_1^{\text{fp}} = -2$ and $C_2^{\text{fp}} = -4\Omega_\phi^{\text{fp}}$): Vacuum solutions where radiation-like effects dominates the nearby evolution of the system, i.e. $w_{\text{eff}}^{\text{fp}} = 1/3$. Scaling solutions for the scalar field.

²Recall that the physical interpretation of these groups is from the point of view of expanding FLRW only. Fixed points corresponding to recollapsing (turnaround) cosmologies or bounce-like events cannot be addressed within our formulation. In addition, there may be fixed points in an expanding FLRW universe that have eluded this classification due to the choice of the dynamical variables being not adequate for them to be properly identified. That may be the case when the auxiliary functions C_1 and C_2 diverge within the configuration space. A way around this issue is discussed in section 4.3.2.

Group 3 ($h^{\text{fp}} = 1$, $\Omega_r^{\text{fp}} = 0$, $C_1^{\text{fp}} \neq -2$ and $C_2^{\text{fp}} = 2C_1^{\text{fp}}\Omega_\phi^{\text{fp}}$): Cosmological singularities where H and its cosmic time derivative diverge but \dot{H}/H^2 (that is C_1) remains finite; e.g. BR singularity.

Group 4 ($h^{\text{fp}} = 1$, $C_1^{\text{fp}} = -2$ and $C_2^{\text{fp}} = -4\Omega_\phi^{\text{fp}}$): Initial cosmological singularities where H and its cosmic time derivative diverge and scaling solutions for the scalar field. It is a radiation dominated regime ($w_{\text{eff}}^{\text{fp}} = 1/3$). E.g. radiation-induced BB singularity.

Group 5 ($h^{\text{fp}} \neq \{0, 1\}$, $\Omega_r^{\text{fp}} = 0$ and $C_1^{\text{fp}} = C_2^{\text{fp}} = 0$): These fixed points necessary obey $\Omega_m^{\text{fp}} = 0$ since $w_{\text{eff}}^{\text{fp}} = -1$. Hence, the scalar field is dominant ($\Omega_\phi^{\text{fp}} = 1$). Moreover, $\Omega_r^{\text{fp}} = \Omega_m^{\text{fp}} = 0$ and $h^{\text{fp}} \in (0, 1)$ imply, in general, that $a^{\text{fp}} \rightarrow \infty$. These represent the asymptotic dS solutions of the theory.

The existence and stability of the above discussed fixed points depend, ultimately, on the choice for the functions K and G . We emphasise that examining the unstable equilibrium points (repellers) and the stable equilibrium points (attractors) offers valuable insight into the cosmological evolution of the model, as trajectories in configuration space are known to evolve from the former to the latter. Nevertheless, the dynamical system approach only provides qualitative information of the solution to the background equations (4.3), (4.4), (4.5), (4.6) and (4.13). This information must be combined with a close inspection of the background equations themselves to obtain as much information as possible on the whole evolution of the system.

Our approach to the dynamical systems analysis of the KGB theory can be summarised as follows. Once the expressions for the functions K and G are specified, the background equations (4.3), (4.4) and (4.13) lead to the auxiliary functions C_1 and C_2 , which, fully characterize the fixed points discussed above; see appendix A. However, definition (4.17) must be inverted for $X = X(h, \Omega_\phi)$ in order to express the autonomous system in the new variables $(h, \Omega_\phi, \Omega_r)$. This suppose the main limiting factor of our approach, as that inversion may not always be possible analytically. In the next sections we present some simple but enlightening examples where this inversion is unambiguous.

4.3 Power law limiting models

For the sake of simplicity in the discussion of the future phenomenology of an expanding FLRW universe in shift-symmetric KGB theories we consider a power law for the functions K and G . That is [168] (see also, for example, references

[346, 434–436])

$$K(X) = c_K X^\alpha \quad \text{and} \quad G(X) = c_G X^\beta, \quad (4.29)$$

being c_K and c_G coupling constants, and α and β the parameters labelling different models. The definition (4.17), then, reduces to

$$3H^2\Omega_\phi = (2\alpha - 1)c_K X^\alpha + 6\sqrt{2}\epsilon c_G \beta H X^{\beta+\frac{1}{2}}. \quad (4.30)$$

Recall that this expression must be inverted for $X = X(h, \Omega_\phi)$, taking also into account the definition (4.19), in order to obtain the closed autonomous system (4.20)–(4.22). The limiting models when only the k -essence function K or the braiding function G are present are discussed below. A proxy example where both functions are present simultaneously is analysed in sections 4.4.

4.3.1 k -essence

We first apply our dynamical systems prescription (4.20)–(4.22) to the well-known power law k -essence theory. This is given by

$$K(X) = c_K X^\alpha \quad \text{and} \quad G(X) = c_G, \quad (4.31)$$

being c_K and c_G constants. Note that $G = \text{const}$ gives rise to a boundary term in the action (2.21) and, therefore, does not contribute to the field equations. From this perspective, one may consider the k -essence theory as a special sub-case of the more general KGB action (2.21). However, it is worth noting that the two scalar field theories have very different properties. This is because second-order derivatives of the metric and scalar field are no longer mixed when G is constant. As a result, some of the most interesting features of the KGB set-up (such as potentially stable phantom crossing) are not present in the k -essence scenario. Still, k -essence represents the most general scalar theory whose action contains up-to first order derivatives of the scalar field and has been extensively explored in a wide variety of cosmological scenarios, from inflation [96, 97] to DE [98, 176–178].

The shift-current (4.7) for this example reads

$$J = \sqrt{2}\alpha\epsilon c_K X^{\alpha-\frac{1}{2}}. \quad (4.32)$$

Comparing this expression with equation (4.14), it follows that $\alpha\epsilon c_K$ and Q_0 should have the same sign. Consequently, the parameter ϵ (i.e. $\text{sgn } \dot{\phi}$) is not allowed to change throughout the evolution of the system. The energy density of the scalar field reads

$$\varrho_\phi = (2\alpha - 1)c_K X^\alpha, \quad (4.33)$$

where $(2\alpha - 1)c_K > 0$ should hold for the energy density to be positive throughout the evolution of the model. From this expression for the energy density it follows that

$$X = \left[\frac{3H_0^2 h^2 \Omega_\phi}{c_K(2\alpha - 1)(1 - h^2)^2} \right]^{\frac{1}{\alpha}}, \quad (4.34)$$

cf. equation (4.30). Please note that the quantity in brackets is always positive as we have demanded $(2\alpha - 1)c_K > 0$ in equation (4.33). The functions C_1 and C_2 then run as follows

$$C_1(\Omega_\phi, \Omega_r) = -\frac{1}{2} \left(3 + \Omega_r + \frac{3\Omega_\phi}{2\alpha - 1} \right), \quad (4.35)$$

$$C_2(\Omega_\phi) = -\frac{6\alpha\Omega_\phi}{2\alpha - 1}, \quad (4.36)$$

see definitions in equations (4.23) and (4.24), respectively. It should be also stressed that these expressions do not depend explicitly on h , c_K or ϵ since they have been completely absorbed into the partial densities Ω_i . Moreover, the function C_2 depends only on the scalar field partial density Ω_ϕ . That is to be expected as equation (4.28) depends only on the kinetic term X when braiding term is absent (cf. [177, 178]).

The fixed points of this model with their stability and physical interpretation are shown in table 4.1. The points labelled as uppercase A_1 down to F_1 are hyperbolic equilibrium points and, therefore, their stability follows from the usual linear theory. Conversely, the calligraphic labels \mathcal{A}_1 , \mathcal{B}_1 and \mathcal{S}_1 represent three sets of non-isolated non-hyperbolic fixed points. For each of these equilibrium sets, one of the eigenvalues of the Jacobian matrix is zero. However, the null eigenvalue corresponds to the eigenvector tangent to the set containing the non-isolated equilibrium points. These are normally hyperbolic equilibrium sets and their stability is given by the real part of the eigenvalues in the remaining directions [270, 280]; see also the introduction to dynamical systems in section 2.4.

Please note that there is only one attractor and one repeller in the configuration space for a given value of the parameter α ; see table 4.1. Physical trajectories in the configuration space start at the corresponding repeller and univocally evolve towards the attractor equilibrium point (i.e. heteroclinic orbits [269, 270, 280]), maybe passing close to a saddle point. It should be emphasised, however, that the classification provided in table 4.1 does not provide any information on the precise evolution of the system. Stated in a different way, it contains only qualitative (but no quantitative) information of the would-be complete solution to background equations (4.3), (4.4), (4.5), (4.6) and (4.13). This information should be combined

Fixed Point	$(h^{\text{fp}}, \Omega_\phi^{\text{fp}}, \Omega_r^{\text{fp}})$	w_ϕ^{fp}	$w_{\text{eff}}^{\text{fp}}$	$\alpha < 0$	$\alpha = 0$	$0 < \alpha < \frac{1}{2}$
A_1 (vacuum)	(0, 0, 0)	$\frac{1}{2\alpha-1}$	0	saddle	saddle	saddle
B_1 (vacuum)	(0, 1, 0)	$\frac{1}{2\alpha-1}$	$\frac{1}{2\alpha-1}$	attractor	-	saddle
C_1 (vacuum)	(0, 0, 1)	$\frac{1}{2\alpha-1}$	$\frac{1}{3}$	saddle	saddle	saddle
D_1 (BB)	(1, 0, 0)	$\frac{1}{2\alpha-1}$	0	saddle	saddle	saddle
E_1 (BB/BR)	(1, 1, 0)	$\frac{1}{2\alpha-1}$	$\frac{1}{2\alpha-1}$	saddle	-	attractor
F_1 (BB)	(1, 0, 1)	$\frac{1}{2\alpha-1}$	$\frac{1}{3}$	repeller	repeller	repeller
\mathcal{A}_1 (vacuum)	$(0, \Omega_\phi^{\text{fp}}, \Omega_r^{\text{fp}})$	$\frac{1}{3}$	$\frac{1}{3}$	-	-	-
\mathcal{B}_1 (BB)	$(1, \Omega_\phi^{\text{fp}}, \Omega_r^{\text{fp}})$	$\frac{1}{3}$	$\frac{1}{3}$	-	-	-
\mathcal{S}_1 (dS)	$(h^{\text{fp}}, 1, 0)$	-1	-1	-	attractor	-

Fixed Point	$(h^{\text{fp}}, \Omega_\phi^{\text{fp}}, \Omega_r^{\text{fp}})$	w_ϕ^{fp}	$w_{\text{eff}}^{\text{fp}}$	$\frac{1}{2} < \alpha < 2$	$\alpha = 2$	$2 < \alpha$
A_1 (vacuum)	(0, 0, 0)	$\frac{1}{2\alpha-1}$	0	attractor	attractor	attractor
B_1 (vacuum)	(0, 1, 0)	$\frac{1}{2\alpha-1}$	$\frac{1}{2\alpha-1}$	saddle	-	saddle
C_1 (vacuum)	(0, 0, 1)	$\frac{1}{2\alpha-1}$	$\frac{1}{3}$	saddle	-	saddle
D_1 (BB)	(1, 0, 0)	$\frac{1}{2\alpha-1}$	0	saddle	saddle	saddle
E_1 (BB/BR)	(1, 1, 0)	$\frac{1}{2\alpha-1}$	$\frac{1}{2\alpha-1}$	repeller	-	saddle
F_1 (BB)	(1, 0, 1)	$\frac{1}{2\alpha-1}$	$\frac{1}{3}$	saddle	-	repeller
\mathcal{A}_1 (vacuum)	$(0, \Omega_\phi^{\text{fp}}, \Omega_r^{\text{fp}})$	$\frac{1}{3}$	$\frac{1}{3}$	-	saddle	-
\mathcal{B}_1 (BB)	$(1, \Omega_\phi^{\text{fp}}, \Omega_r^{\text{fp}})$	$\frac{1}{3}$	$\frac{1}{3}$	-	repeller	-
\mathcal{S}_1 (dS)	$(h^{\text{fp}}, 1, 0)$	-1	-1	-	-	-

Table 4.1: Classification and linear stability of the fixed points of the model (4.31). A superscript “fp” denotes evaluation at the fixed point whereas a horizontal bar indicates that the corresponding fixed point does not exist. The calligraphic characters \mathcal{A}_1 , \mathcal{B}_1 and \mathcal{S}_1 label normally hyperbolic equilibrium sets. The condition $\Omega_\phi^{\text{fp}} + \Omega_r^{\text{fp}} = 1$ holds for \mathcal{A}_1 and \mathcal{B}_1 . In addition, h^{fp} may take any values (different from 0 or 1) in \mathcal{S}_1 . To enhance the readability of the table, the cases with $\alpha < 1/2$ are presented at the top of the page, while the remaining cases ($\alpha > 1/2$) are positioned just below.

with a close inspection of the background equations themselves to obtain as much information as possible on the particular dynamics of each trajectory.

Recall that we have focused our analysis on expanding FLRW only and, therefore, the physical interpretation of the points in table 4.1 is deduced according to that ansatz. Equilibrium points corresponding to bounce or turnaround-like events, if any, cannot be described within this approach³. According to this interpretation, and taking also into account the background equations (4.3), (4.4), (4.5), (4.6) and (4.13), it follows that the equilibrium points A_1 , B_1 and C_1 , and the equilibrium set \mathcal{A}_1 correspond to vacuum solutions where all the components of the universe are, eventually, redshifted away with the expansion. Moreover, \mathcal{A}_1 contains scaling solutions where the scalar field mimics radiation. The points A_1 and B_1 belong to group 1 in the classification discussed in section 4.2.2. Conversely, C_1 and \mathcal{A}_1 are part of group 2.

The fixed point D_1 may be interpreted as an initial matter-induced BB singularity where only some trajectories (those where radiation is absent in the early universe) may begin at D_1 if matter dominates over the scalar field in the asymptotic past of the system. However, since a non-trivial radiation content will always dominate over matter at early times, D_1 necessarily acts as a saddle point in the configuration space. This point belongs to group 3.

At the equilibrium point E_1 the scalar field drives the divergence of both H and \dot{H} . This may have different physical interpretations depending on the moment in the cosmological expansion when this regime is reached. Since the scalar field is the dominant component at E_1 , then the approximation

$$3H^2 \approx \mu_1 \left(\frac{a}{a_0} \right)^{-\frac{6\alpha}{2\alpha-1}}, \quad (4.37)$$

holds true, where

$$\mu_1 := (2\alpha - 1)c_K \left(\frac{Q_0}{\sqrt{2\epsilon\alpha c_K}} \right)^{\frac{2\alpha}{2\alpha-1}} \quad (4.38)$$

is a positive constant since Q_0 and $\epsilon\alpha c_K$ have the same sign (compare (4.14) and (4.32)), and $(2\alpha - 1)c_K$ is positive (i.e. $\varrho_\phi > 0$). For $\alpha \in (1/2, 2)$ the scalar field dominates over radiation in the very early universe, thus, leading to the divergence of the Hubble rate and its time derivative as $a \rightarrow 0$. Hence, a scalar-field-induced BB singularity takes place. On the other hand, if $\alpha \in (0, 1/2)$, the Hubble rate becomes proportional to a positive power of the scale factor. It is a well-known result that in this situation a , H and \dot{H} blow-up in a finite cosmic

³However, each of the points in table 4.1 would have an exact counterpart in a monotonically contracting cosmos where $h^{\text{fp}} \rightarrow -h^{\text{fp}}$ and with precisely the opposite stability.

time (see appendix B for a justification of this claim). Consequently, the model (4.31) entails a BR singularity when $\alpha \in (0, 1/2)$. In fact, this is the only future attractor in the configuration space for that set of values of α ; see table 4.1. For the rest of the α -line, the exponent in equation (4.37) is negative but greater than -4 (radiation dominance). This leads to saddle configurations that can be interpreted in the same fashion as for D_1 . The equilibrium point E_1 belongs to group 3 in the discussion of the previous section.

F_1 represents a radiation dominated BB singularity. It naturally acts as a repeller in the configuration space except for those values of α for which the scalar field dominates at the very early universe. An interesting subcase of this event is when $\alpha = 2$, in this scenario the scalar field scales exactly as radiation. This scaling solution also corresponds to a radiation-induced BB singularity; see \mathcal{B}_1 in table 4.1. Both of these scenarios belong to group 4 in our previous classification.

It should be noted that $\alpha = 0$ corresponds to the standard Λ CDM model where the role of the cosmological constant is portrayed by the coupling constant c_K ; that is $\Lambda = -c_K$ where $c_K < 0$ (since ϱ_ϕ positive). Therefore, the expansion history of the model for $\alpha = 0$ would be that of Λ CDM. That is, the system would evolve towards a future dS state⁴ provided that c_K is not null (see \mathcal{S}_1 in table 4.1). The scalar field dominated fixed points B_1 and E_1 are not present in this case since they would correspond to $c_K = 0$ (i.e. no scalar field) and $c_K \rightarrow \infty$ (unphysical), respectively.

Finally, it should be also mentioned that for $\alpha = 1/2$ the scalar field energy density (4.33) is trivial. Please note that having a kinetic term of the type \sqrt{X} in the action strongly resembles Cuscuton gravity [437]. However, the shift-symmetry here assumed prevents from having potential-like terms for the scalar field, which are responsible for the non-trivial behaviour of the *cuscuta* in homogeneous and isotropic backgrounds [438]. This sets the difference between this model and Cuscuton gravity. In our shift-symmetric case, the universe is filled with dust and radiation only for $\alpha = 1/2$. This scenario is not included in table 4.1 as our interest resides mainly in the DE phenomenology coming from the scalar field.

4.3.2 Proxy braiding model

A simple proxy model of the KGB theory is that when only the G function is present in the action (4.2). For a power law prescription, this reads [3]

$$K(X) = 0 \quad \text{and} \quad G(X) = c_G X^\beta, \quad (4.39)$$

⁴This is indeed the only dS solution for the power law kinetic k-essence model at hand.

being c_G a coupling constant and β the parameter labelling different models; see also reference [2]. In this proxy scenario, the shift-current (4.7) reduces to

$$J = 6\beta c_G H X^\beta. \quad (4.40)$$

As a result, the energy density of the scalar field reads

$$\varrho_\phi = 6\sqrt{2}\epsilon c_G \beta H X^{\beta+\frac{1}{2}}, \quad (4.41)$$

where $\beta\epsilon c_G H \geq 0$ should hold for this energy density to be non-negative. In an expanding universe ($H > 0$), this condition implies that ϵ cannot change its sign throughout the evolution of the system. Reversing equation (4.41) for X leads to

$$X = \left[\frac{H_0 h \Omega_\phi}{2\sqrt{2}\beta\epsilon c_G (1-h^2)} \right]^{\frac{2}{2\beta+1}}, \quad (4.42)$$

where the quantity in brackets is clearly positive provided that the aforementioned condition holds; compare also with equation (4.30) for $c_K \equiv 0$.

The auxiliary functions C_1 and C_2 for this model read

$$C_1(\Omega_\phi, \Omega_r) = -\frac{2\beta\Omega_r + 6\beta + 3\Omega_\phi}{4\beta + \Omega_\phi}, \quad (4.43)$$

$$C_2(\Omega_\phi, \Omega_r) = \Omega_\phi \frac{\Omega_r - 3 - 12\beta - 3\Omega_\phi}{4\beta + \Omega_\phi}, \quad (4.44)$$

see definitions in equations (4.23) and (4.24), respectively. As for the kinetic k -essence model, these functions do not explicitly depend on h , c_G or ϵ since they have been completely absorbed in the definitions of the partial densities. However, now the function C_2 depends also on the external matter content of the theory, namely⁵ Ω_r . Moreover, this function is related to w_ϕ and, therefore, to the evolution of the scalar field. This is a direct manifestation of the *kinetic braiding* in the theory [40].

The fixed points of this model are shown in table 4.2. Parallel to the notation in the previous section, the points labelled in uppercase A_2 down to F_2 represent hyperbolic equilibrium points of the system and their stability follows from the usual linear theory. The calligraphic labels \mathcal{A}_2 , \mathcal{B}_2 and \mathcal{S}_2 denote normally hyperbolic equilibrium sets. The new G_2 and C_2 entries in table 4.2 represent events that have eluded our analysis because of the choice for the dynamical variables being not adequate for them to be properly identified as equilibrium configurations of the system. Nevertheless, their existence and stability follow directly from the background equations (a discussion we return to below). Please note that this was

Fixed Point	$(h^{\text{fp}}, \Omega_\phi^{\text{fp}}, \Omega_r^{\text{fp}})$	w_ϕ^{fp}	$w_{\text{eff}}^{\text{fp}}$	$\beta < -\frac{1}{2}$	$\beta = -\frac{1}{2}$	$-\frac{1}{2} < \beta < -\frac{1}{4}$	$\beta = -\frac{1}{4}$
A_2 (vacuum)	$(0, 0, 0)$	$\frac{1}{4\beta}$	0	saddle	saddle	saddle	saddle
B_2 (vacuum)	$(0, 1, 0)$	$\frac{1}{4\beta+1}$	$\frac{1}{4\beta+1}$	attractor	attractor	saddle	-
C_2 (vacuum)	$(0, 0, 1)$	$\frac{1}{6\beta}$	$\frac{1}{3}$	saddle	saddle	saddle	saddle
D_2 (BB)	$(1, 0, 0)$	$\frac{1}{4\beta}$	0	saddle	saddle	saddle	saddle
E_2 (BB/BR)	$(1, 1, 0)$	$\frac{1}{4\beta+1}$	$\frac{1}{4\beta+1}$	saddle	-	attractor	-
F_2 (BB)	$(1, 0, 1)$	$\frac{1}{6\beta}$	$\frac{1}{3}$	repeller	repeller	repeller	repeller
G_2 (BF)	$(1, 1, 0)$	$-\infty$	$-\infty$	-	-	-	attractor*
\mathcal{A}_2 (vacuum)	$(0, \Omega_\phi^{\text{fp}}, \Omega_r^{\text{fp}})$	$\frac{1}{3}$	$\frac{1}{3}$	-	-	-	-
\mathcal{B}_2 (BB)	$(1, \Omega_\phi^{\text{fp}}, \Omega_r^{\text{fp}})$	$\frac{1}{3}$	$\frac{1}{3}$	-	-	-	-
\mathcal{C}_2 (sudden)	$(h^{\text{fp}}, -4\beta, \Omega_r^{\text{fp}})$	$-\infty$	$-\infty$	-	-	-	-
\mathcal{S}_2 (dS)	$(h^{\text{fp}}, 1, 0)$	-1	-1	-	attractor	-	-

Fixed Point	$(h^{\text{fp}}, \Omega_\phi^{\text{fp}}, \Omega_r^{\text{fp}})$	w_ϕ^{fp}	$w_{\text{eff}}^{\text{fp}}$	$-\frac{1}{4} < \beta < 0$	$0 < \beta < \frac{1}{2}$	$\beta = \frac{1}{2}$	$\frac{1}{2} < \beta$
A_2 (vacuum)	$(0, 0, 0)$	$\frac{1}{4\beta}$	0	saddle	attractor	attractor	attractor
B_2 (vacuum)	$(0, 1, 0)$	$\frac{1}{4\beta+1}$	$\frac{1}{4\beta+1}$	saddle	saddle	-	saddle
C_2 (vacuum)	$(0, 0, 1)$	$\frac{1}{6\beta}$	$\frac{1}{3}$	saddle	saddle	-	saddle
D_2 (BB)	$(1, 0, 0)$	$\frac{1}{4\beta}$	0	saddle	saddle	saddle	saddle
E_2 (BB/BR)	$(1, 1, 0)$	$\frac{1}{4\beta+1}$	$\frac{1}{4\beta+1}$	repeller	repeller	-	saddle
F_2 (BB)	$(1, 0, 1)$	$\frac{1}{6\beta}$	$\frac{1}{3}$	repeller	saddle	-	repeller
G_2 (BF)	$(1, 1, 0)$	$-\infty$	$-\infty$	-	-	-	-
\mathcal{A}_2 (vacuum)	$(0, \Omega_\phi^{\text{fp}}, \Omega_r^{\text{fp}})$	$\frac{1}{3}$	$\frac{1}{3}$	-	-	saddle	-
\mathcal{B}_2 (BB)	$(1, \Omega_\phi^{\text{fp}}, \Omega_r^{\text{fp}})$	$\frac{1}{3}$	$\frac{1}{3}$	-	-	repeller	-
\mathcal{C}_2 (sudden)	$(h^{\text{fp}}, -4\beta, \Omega_r^{\text{fp}})$	$-\infty$	$-\infty$	attractor*	-	-	-
\mathcal{S}_2 (dS)	$(h^{\text{fp}}, 1, 0)$	-1	-1	-	-	-	-

Table 4.2: Classification and linear stability of the fixed points of the model (4.39). The calligraphic characters \mathcal{A}_2 , \mathcal{B}_2 , \mathcal{C}_2 and \mathcal{S}_2 label sets of non-isolated fixed points where in the latter h^{fp} may take any values (different from 0 or 1). In addition, $\Omega_\phi^{\text{fp}} + \Omega_r^{\text{fp}} = 1$ holds for \mathcal{A}_2 and \mathcal{B}_2 , and $\Omega_r^{\text{fp}} \in [0, 1 + 4\beta]$ for \mathcal{C}_2 . The starred quantities indicate fixed points that have eluded our dynamical system analysis because of the choice of the dynamical variables but whose existence and stability follows directly from the background equations. For the sake of presentation, the table has been divided into two parts: the upper portion displays the stability for $\beta < -1/4$, while the lower portion encompasses the cases with $\beta > -1/4$.

not the case in the k -essence model (4.31), where all fixed points (in expanding FLRW) were perfectly captured within our description.

The physical interpretation of the fixed points in table 4.2 is analogous to that of the kinetic k -essence scenario discussed before, where we recall again that the dynamical system analysis provides only qualitative information that must be combined with a close inspection of the background equations (4.3), (4.4), (4.5), (4.6) and (4.13) to obtain as much information as possible on the particular dynamics of each trajectory in the configuration space. Thus, A_2 , B_2 , C_2 and \mathcal{A}_2 represent vacuum solutions in an expanding universe. The points A_2 and B_2 belong to group 1, whereas C_2 and \mathcal{A}_2 to group 2. The label D_2 (group 3) denotes a saddle configuration where a matter-induced BB takes place. A radiation-induced BB corresponds to F_2 and \mathcal{B}_2 , where for the latter the scalar field scales exactly as radiation. Both fixed points belong to group 4.

As in the previous section, E_2 (group 3) may have different interpretations depending on the parameter β . Since the scalar field dominates over dust and radiation, and taking also into account equation (4.14), the Friedmann equation (4.3) in an expanding universe ($H > 0$) reduces to

$$H \approx \mu_2 \left(\frac{a}{a_0} \right)^{-3 \frac{2\beta+1}{4\beta+1}}, \quad (4.45)$$

being

$$\mu_2 := \left(\frac{\sqrt{2}}{3} \epsilon Q_0 \right)^{\frac{2\beta}{4\beta+1}} \left(\frac{Q_0}{6\beta c_G} \right)^{\frac{1}{4\beta+1}} \quad (4.46)$$

a positive constant since ϵQ_0 and $Q_0/\beta c_G$ are positive⁶. When $\beta \in (-1/4, 1/2)$, the scalar field dominates over radiation as $a \rightarrow 0$. This results in a scalar-field-induced BB. On the other hand, if $\beta \in (-1/2, -1/4)$ the exponent becomes positive and, therefore, a future BR singularity takes place; see appendix B. For the rest of the β -line, E_2 corresponds to saddle configurations where ϱ_ϕ either dominates or not over matter when $a \rightarrow 0$.

The case of $\beta = 0$ is not portrayed in table 4.2 since $G = \text{const}$ gives a boundary term in the action (2.21) and, therefore, the corresponding model would contain dust and radiation only (recall that $K = 0$ for the model at hand). Another critical value for β is that of $-1/2$. In that case, the energy density of the scalar

⁵Recall that Ω_m has been eliminated from the system with the Friedmann constraint (4.18).

⁶The condition $\epsilon c_G \beta > 0$ follows from demanding ϱ_ϕ to be non-negative, whereas $\text{sgn}(Q_0) = \text{sgn}(\beta \epsilon c_G)$ comes from comparing equations (4.14) and (4.40). Combining these two conditions, it is straightforward to obtain that ϵQ_0 and $Q_0/\beta c_G$ are positive. Hence, the constant μ_2 is well-defined and positive.

field depends only on the Hubble rate; see equation (4.41). Thus, as matter and radiation are redshifted away the Hubble rate converges to a constant value given by $H = -\sqrt{2}\epsilon c_G$, where $\epsilon c_G \leq 0$; cf. $\beta = -1/2$ in equation (4.45). This solution corresponds to the dS fixed point of the system (group 5) if ϵ is not null; see \mathcal{S}_2 in table 4.2. The vacuum equilibrium point B_2 (group 1) is obtained if $\epsilon = 0$ in the future. Please note that B_2 and \mathcal{S}_2 lined-up in a set of normally hyperbolic fixed points. We have represented them separately in table 4.2 (when $\beta = -1/2$) only to facilitate their physical interpretation. Therefore, for this value of β all trajectories in the configuration space will evolve from F_2 to the B_2 - \mathcal{S}_2 equilibrium line. Also note that the scalar field dominated fixed point E_2 is not present for $\beta = -1/2$ in an expanding universe since it would correspond to $c_G \rightarrow \infty$ (unphysical).

Please note that special attention should be paid to $\Omega_\phi = -4\beta$, moment at which the denominator in equations (4.43) and (4.44) cancels. This takes place in the physical configuration space whenever $\beta \in [-1/4, 0)$. In that case the dynamical system portrayed by the auxiliary functions C_1 and C_2 is potentially ill-defined and, therefore, fixed points corresponding to this value for Ω_ϕ , if any, would be hardly studied within this formulation. Nevertheless, the behaviour of the model at this moment can be directly inferred from the Friedmann and Raychaudhuri equations. Consider first the case of $\beta = -1/4$, which corresponds to the dynamical system (4.20)-(4.22) being potentially ill-defined at $\Omega_\phi = 1$. For this value of the exponent β , the Friedmann equation (4.3) reduces to

$$\left[1 - \Omega_\phi^{(0)} \left(\frac{a}{a_0}\right)^3\right] \frac{H^2}{H_0^2} = \Omega_r^{(0)} \left(\frac{a}{a_0}\right)^{-4} + \Omega_m^{(0)} \left(\frac{a}{a_0}\right)^{-3}, \quad (4.47)$$

being $\Omega_r^{(0)}$, $\Omega_m^{(0)}$ and $\Omega_\phi^{(0)}$ the present value of the partial densities for radiation, matter and the scalar field, respectively. For an expanding geometry, the expression in brackets on the left-hand side vanishes at a finite scale factor, namely $a_s^3 := a_0^3/\Omega_\phi^{(0)}$. Nevertheless, since the right-hand side of the preceding equation is different from zero whenever the scale factor a is finite, then, the Hubble rate necessarily diverge when the bracket vanishes. Similarly, the Raychaudhuri equation (4.4) simplifies to

$$\left[1 - \Omega_\phi^{(0)} \left(\frac{a}{a_0}\right)^3\right] \frac{\dot{H}}{H_0^2} = \frac{3}{2}\Omega_\phi^{(0)} \left(\frac{a}{a_0}\right)^3 \frac{H^2}{H_0^2} - \frac{1}{2} \left[4\Omega_r^{(0)} \left(\frac{a}{a_0}\right)^{-4} + 3\Omega_m^{(0)} \left(\frac{a}{a_0}\right)^{-3}\right], \quad (4.48)$$

for $\beta = -1/4$, which implies that \dot{H} also diverges when the observable universe reaches the maximum size a_s . Moreover, both H and \dot{H} diverge at a finite cosmic time⁷. In addition, the scalar field exhibits strong phantom behaviour near a_s .

⁷This follows from the fact that $1/aH$ is always bounded on the compact $a \in [0, a_s]$. Hence,

The EOS parameters w_{eff} and w_ϕ even diverge to minus infinity when H and \dot{H} explode. This behaviour corresponds to a BF singularity; see references [218, 219] and, for instance, the type III singularities in the classification of reference [134]. In fact, this BF singularity takes place for an expanding universe regardless the values for the initial partial densities. Therefore, this cosmic singularity acts as a genuine attractor in the theory even though our characterization of the dynamical system by means of the variables h , Ω_ϕ and Ω_r is not well-suited for describing this event. For the sake of completeness, this attractor has been added to table 4.2 under the label G_2 .

A similar line of reasoning with the Friedmann and Raychaudhuri equations,

$$\frac{H^2}{H_0^2} = \Omega_r^{(0)} \left(\frac{a}{a_0}\right)^{-4} + \Omega_m^{(0)} \left(\frac{a}{a_0}\right)^{-3} + \Omega_\phi^{(0)} \left(\frac{a}{a_0}\right)^{-3\frac{2\beta+1}{2\beta}} \left(\frac{H}{H_0}\right)^{-\frac{1}{2\beta}}, \quad (4.49)$$

$$\left[1 + \frac{\Omega_\phi^{(0)}}{4\beta} \left(\frac{a}{a_0}\right)^{-3\frac{2\beta+1}{2\beta}} \left(\frac{H}{H_0}\right)^{-\frac{4\beta+1}{2\beta}}\right] \frac{\dot{H}}{H_0^2} = -2\Omega_r^{(0)} \left(\frac{a}{a_0}\right)^{-4} - \frac{3}{2}\Omega_r^{(0)} \left(\frac{a}{a_0}\right)^{-3} - \frac{3\Omega_\phi^{(0)}(2\beta+1)}{4\beta} \left(\frac{a}{a_0}\right)^{-3\frac{2\beta+1}{2\beta}} \left(\frac{H}{H_0}\right)^{-\frac{1}{2\beta}}, \quad (4.50)$$

respectively, concludes that \dot{H} diverge at a finite value for a and H whenever $\beta \in (-1/4, 0)$. That occurs when the bracket in the left-hand side of the latter equation cancels, which corresponds to $\Omega_\phi = -4\beta$ in terms of our dynamical system variables. Moreover, the divergence occurs at a finite value of the cosmic time since $1/aH$ is always bounded; see footnote 7. This behaviour corresponds to that of a sudden singularity [220] (see also type II singularities in the classification of reference [134]). Since an expanding system always evolves towards this scenario regardless the choice for the initial partial densities, this event has been added to table 4.2 as an attractor in the corresponding configuration space; see \mathcal{C}_2 in table 4.2. It should be also mentioned that two repellers are simultaneously present when $\beta \in (-1/4, 0)$. This is because \mathcal{C}_2 acts as a separatrix dividing the configuration space into two separated parts, where each of the halves contains one of the repellers. The heteroclinic orbits in each part of the configuration space will begin at the corresponding repeller (E_2 or F_2) and evolve towards \mathcal{C}_2 .

For each particular choice of model parameters, a different phase portrait would be obtained displaying the corresponding critical points, as shown in table 4.2.

the integral

$$\int_0^{a_s} \frac{da}{aH} = \int_0^{t_s} dt$$

is finite.

See, for instance, appendix C for an example corresponding to a model featuring a BR attractor in the configuration space. Please let us highlight that, to the best of our knowledge, this is the first time a BR, a BF or a sudden cosmic singularity have been explicitly described in the shift-symmetric sector of the KGB theory. These results suggest that the future phenomenology of the KGB theory may be richer than previously thought. Furthermore, the presence of finite-size singularities reinforces our initial claim that $J = 0$ is not, in general, an exhaustive characterization of all the possible future attractors for an expanding universe in the shift-symmetric KGB theory. This is because the observable universe reaches a maximum size and, therefore, in view of expression (4.14), $J \neq 0$ on the future attractor provided that the shift-charge Q_0 is non-trivial.

4.4 A kinetic gravity braiding model

As we mentioned before, the inversion of equation (4.17) to obtain $X = X(\Omega_\phi, H)$ is the main limiting factor in our formulation of the dynamical system. So far, we have only addressed marginal power law examples where one of the KGB functions was trivial. We present now an example of the complete KGB theory where the inversion of equation (4.30) is still approachable. This model is given by [2]

$$K(X) = c_K X^\alpha \quad \text{and} \quad G(X) = c_G X^{\alpha - \frac{1}{2}}, \quad (4.51)$$

being c_K and c_G coupling constants. Keeping both constants different from unity may seem artificially tedious, since it is always possible to redefine the scalar field ϕ in such a way that one of the coupling constants gets reabsorbed. Nevertheless, we shall keep both of them for the sake of the argument. Also note that the model (4.51) is a subclass of the extended Galileon studied in references [168, 346, 435]. The expression for the shift-current (4.7) reduces to

$$J = \left[\sqrt{2\alpha\epsilon} c_K + 3(2\alpha - 1)c_G H \right] X^{\alpha - \frac{1}{2}}. \quad (4.52)$$

As a result, the energy density of the scalar field runs as follows

$$\varrho_\phi = (2\alpha - 1) \left(c_K + 3\sqrt{2\epsilon} c_G H \right) X^\alpha. \quad (4.53)$$

Demanding this energy density to be positive, at least when the scalar is dominant, is not so straightforward as for the previous models. This is because the parameter ϵ is not fixed (as it was in the previous examples) and, therefore, it could change its sign throughout the evolution of the system. We explore the necessary conditions for this energy density to be positive when the scalar field is dominant in section 4.4.2.

Taking into account the definitions (4.17) and (4.19), equation (4.30) yields

$$X = \left[\frac{3H_0^2 \gamma h^2 \Omega_\phi}{(2\alpha - 1)c_K (1 - h^2) (\gamma(1 - h^2) + h)} \right]^{\frac{1}{\alpha}}, \quad (4.54)$$

where $\gamma := c_K / (3\sqrt{2}\epsilon H_0 c_G)$ is a dimensionless quantity introduced for the sake of the notation. The corresponding functions C_1 and C_2 read [2]

$$C_1 = - \frac{(2\gamma\alpha(1 - h^2) + (2\alpha - 1)h) (\gamma(1 - h^2) + h) ((2\alpha - 1)(3 + \Omega_r) + 3\Omega_\phi)}{(2\alpha - 1) \left[4\alpha (\gamma(1 - h^2) + h)^2 - 2h (\gamma(1 - h^2) + h) + h^2 \Omega_\phi \right]}, \quad (4.55)$$

$$C_2 = -\Omega_\phi \times \frac{24\alpha^2 (\gamma(1 - h^2) + h)^2 - 12\alpha h (\gamma(1 - h^2) + h) + (2\alpha - 1)h^2 (3\Omega_\phi - \Omega_r - 3)}{(2\alpha - 1) \left[4\alpha (\gamma(1 - h^2) + h)^2 - 2h (\gamma(1 - h^2) + h) + h^2 \Omega_\phi \right]}, \quad (4.56)$$

where the interplay between both K and G functions has now introduced an explicit dependence on h . In addition, there is also an explicit dependence on the parameter γ . That should not be surprising as in this scenario there are two coupling constants for the scalar field and, therefore, the dynamics of the system is expected to depend on their ratio. Also note that these expressions for the functions C_1 and C_2 reduce to those presented in section 4.3.1 when $\gamma \rightarrow \infty$ (i.e. $c_G \rightarrow 0$), and to those in section 4.3.2 when $\gamma \rightarrow 0$ (that is $c_K \rightarrow 0$), as one would naturally expect.

4.4.1 The fixed points

The fixed points of the system are listed in table 4.3. Following the previous notation, the fixed points labelled with the uppercase letters A_3 down to S_3^2 are hyperbolic equilibrium points whose stability has been deduced linearising the dynamical equations (4.20)-(4.22). While the calligraphic letters \mathcal{A}_3 and \mathcal{B}_3 denote normally hyperbolic equilibrium sets. Note that $\alpha = 1/2$ is intentionally not listed in table 4.3 for the same reason as in section 4.3.1: even though it may seem similar to Cuscuton gravity [437, 438], the absence of a potential-like term due to the shift-symmetry forces the scalar field not to contribute at all to the dynamics of the model. The case of $\alpha = 0$ is not listed in table 4.3 either, as it reduces to the model (4.39) with $\beta = -1/2$ plus a cosmological constant ($\Lambda = -c_K$) and, therefore, the dynamical structure is qualitatively equivalent to that presented in the corresponding column of table 4.2.

Fixed Point	$(h^{\text{fp}}, \Omega_\phi^{\text{fp}}, \Omega_{\text{r}}^{\text{fp}})$	w_ϕ^{fp}	$w_{\text{eff}}^{\text{fp}}$	$\alpha < 0$	$0 < \alpha < \frac{1}{4}$	$\alpha = \frac{1}{4}$	$\frac{1}{4} < \alpha < \frac{1}{2}$
A ₃ (vacuum)	(0, 0, 0)	$\frac{1}{2\alpha-1}$	0	saddle	saddle	saddle	saddle
B ₃ (vacuum)	(0, 1, 0)	$\frac{1}{2\alpha-1}$	$\frac{1}{2\alpha-1}$	attractor	saddle	saddle	saddle
C ₃ (vacuum)	(0, 0, 1)	$\frac{1}{2\alpha-1}$	$\frac{1}{3}$	saddle	saddle	saddle	saddle
D ₃ (BB)	(1, 0, 0)	$\frac{1}{4\alpha-2}$	0	saddle	saddle	saddle	saddle
E ₃ (BB/BR)	(1, 1, 0)	$\frac{1}{4\alpha-1}$	$\frac{1}{4\alpha-1}$	saddle	attractor	-	repeller
F ₃ (BB)	(1, 0, 1)	$\frac{1}{6\alpha-3}$	$\frac{1}{3}$	repeller	repeller	repeller	repeller
S ₃ ¹ (dS)	$(h_1, 1, 0)$	-1	-1	attractor	attractor	attractor	attractor
S ₃ ² (dS)	$(h_2, 1, 0)$	-1	-1	saddle	attractor	attractor	attractor
\mathcal{A}_3 (vacuum)	$(0, \Omega_\phi^{\text{fp}}, \Omega_{\text{r}}^{\text{fp}})$	$\frac{1}{3}$	$\frac{1}{3}$	-	-	-	-
\mathcal{B}_3 (BB)	$(1, \Omega_\phi^{\text{fp}}, \Omega_{\text{r}}^{\text{fp}})$	$\frac{1}{3}$	$\frac{1}{3}$	-	-	-	-

Fixed Point	$(h^{\text{fp}}, \Omega_\phi^{\text{fp}}, \Omega_{\text{r}}^{\text{fp}})$	$\frac{1}{2} < \alpha < 1$	$\alpha = 1$	$1 < \alpha < 2$	$\alpha = 2$	$2 < \alpha$
A ₃ (vacuum)	(0, 0, 0)	attractor	attractor	attractor	attractor	attractor
B ₃ (vacuum)	(0, 1, 0)	saddle	saddle	saddle	-	saddle
C ₃ (vacuum)	(0, 0, 1)	saddle	saddle	saddle	-	saddle
D ₃ (BB)	(1, 0, 0)	saddle	saddle	saddle	saddle	saddle
E ₃ (BB/BR)	(1, 1, 0)	repeller	-	saddle	saddle	saddle
F ₃ (BB)	(1, 0, 1)	saddle	-	repeller	repeller	repeller
S ₃ ¹ (dS)	$(h_1, 1, 0)$	attractor	attractor	attractor	attractor	attractor
S ₃ ² (dS)	$(h_2, 1, 0)$	saddle	saddle	saddle	saddle	saddle
\mathcal{A}_3 (vacuum)	$(0, \Omega_\phi^{\text{fp}}, \Omega_{\text{r}}^{\text{fp}})$	-	-	-	saddle	-
\mathcal{B}_3 (BB)	$(1, \Omega_\phi^{\text{fp}}, \Omega_{\text{r}}^{\text{fp}})$	-	repeller	-	-	-

Table 4.3: Classification and linear stability of the fixed points of the model (4.51). A superscript “fp” denotes evaluation at the fixed point whereas a horizontal bar indicates that the corresponding fixed point does not exist. The calligraphic characters \mathcal{A}_3 and \mathcal{B}_3 label normally hyperbolic equilibrium sets where the condition $\Omega_\phi^{\text{fp}} + \Omega_{\text{r}}^{\text{fp}} = 1$ holds. The expressions for h_1 and h_2 can be found in equations (4.59) and (4.60), respectively. To enhance the readability of the table, the cases with $\alpha < 1/2$ are presented at the top of the page, while the remaining scenarios ($\alpha > 1/2$) are positioned just below.

The events labelled as A_3 , B_3 , C_3 and \mathcal{A}_3 represent vacuum solutions. The latter two belong to group 1, whereas the former two are members of group 2. Moreover, D_3 (group 3) admits the same physical interpretation as for D_1 and D_2 ; cf. tables 4.1 and 4.2, respectively.

On the other hand, equations (4.14), (4.52) and (4.53) allow for re-expressing the scalar field energy density as a function of a and H only. Since this is the dominant component at E_3 (group 3), and expanding ϱ_ϕ for large values of the Hubble rate, the Friedmann equation (4.3) simplifies (asymptotically in the H -line) as [2]

$$H \approx \mu_3 \left(\frac{a}{a_0} \right)^{-\frac{6\alpha}{4\alpha-1}}, \quad (4.57)$$

being

$$\mu_3 := \left(\frac{1}{3} \right)^{\frac{2\alpha-1}{4\alpha-1}} \left(\frac{H_0 \gamma}{(2\alpha-1)c_K} \right)^{\frac{1}{4\alpha-1}} \left(\frac{\sqrt{2}Q_0}{\epsilon} \right)^{\frac{2\alpha}{4\alpha-1}} \quad (4.58)$$

a positive constant (see section 4.4.2). The exponent in expression (4.57) becomes positive for $\alpha \in (0, 1/4)$, which signals a future BR singularity; see appendix B. Indeed, E_3 behaves as an attractor in the configuration space for those values, see table 4.3. Conversely, for $\alpha \in (1/4, 1)$ the scalar field dominates over radiation in the past. In that case, E_3 represents a scalar-field-induced BB. For the other values of α , this equilibrium point features saddle configurations that can be interpreted in the same way as for D_3 .

A radiation-induced BB singularity takes place at F_3 and \mathcal{B}_3 , where for the latter the scalar field contributes to the total radiation content of the universe (scaling solutions). These equilibrium points are part of group 4 in our previous classification.

A new feature of this model is the presence of h in the functions C_1 and C_2 . This allows for different solutions corresponding to future dS states in contrast with the previously discussed models where only one dS attractor was found for a specific value of the corresponding parameter; see tables 4.1 and 4.2. These equilibrium points (group 5) correspond to different solutions to $C_1^{\text{fp}} = C_2^{\text{fp}} = 0$ and $\Omega_\phi^{\text{fp}} = 1$ for $h^{\text{fp}} < 1$. According to the structure of the function C_1 , one such possibility is when the first parenthesis in the numerator of equation (4.55) cancels. This occurs at [2]

$$h_1 = \frac{2\alpha-1}{4\alpha\gamma} \left[1 \pm \sqrt{1 + \left(\frac{4\alpha\gamma}{2\alpha-1} \right)^2} \right]. \quad (4.59)$$

However, only the negative branch in the preceding expression satisfies the restriction $h_1 \in (0, 1)$ either when $\gamma > 0$ and $\alpha \in (0, 1/2)$, or $\gamma < 0$ and $\alpha \notin [0, 1/2]$. This dS solution has been labelled as \mathcal{S}_3^1 in table 4.3.

Another solution representing a future dS state is that when the second parenthesis in the numerator of C_1 vanishes. This is when h converges to [2]

$$h_2 = \frac{1}{2\gamma} \left(1 \pm \sqrt{1 + 4\gamma^2} \right), \quad (4.60)$$

where only the negative branch belong to the physical configuration space, i.e. $h_2 \in (0, 1)$, if γ is negative. This event has been assigned the label \mathcal{S}_3^2 in table 4.3.

In a similar way to the model (4.39) previously discussed, the dynamical system is potentially ill-defined when the denominator of the auxiliary functions C_1 and C_2 vanishes. In an expanding universe, it can be shown analytically that this is not the case if γ is positive and $\alpha < 0$ or $\alpha > 1/2$. However, restricting γ to be positive may not always be viable given that ϵ could change its sign during the evolution of the system when the scalar field is subdominant. On the contrary, if the scalar field dominates, this parameter can be unambiguously fixed; see section 4.4.2. Unfortunately, the complexity of the denominator in equations (4.55) and (4.56) does not admit an analytic analysis with the background equations like we have done for the model (4.39). Consequently, fixed points of the system in the region of the configuration space where this denominator cancels, if any, remain beyond the scope of this formulation for the dynamical system.

4.4.2 Conditions for the positivity of the scalar field energy density

In this section we discuss the restrictions on c_K , c_G and ϵ for the energy density (4.53) to be positive at least when the scalar field is dominant. In practice, we focus our analysis to the evolution of the system around the equilibrium points where $\Omega_\phi^{\text{fp}} = 1$ in table 4.3. The results are summarized in table 4.4. These are:

Vacuum solutions These are characterized by $h^{\text{fp}} = 0$. Hence, demanding the scalar field energy density (4.53) to be positive at $H \approx 0$ implies $(2\alpha - 1)c_K > 0$. This condition applies to B_3 and \mathcal{A}_3 in table 4.3. In addition, comparing expressions (4.14) and (4.52), it follows that $\epsilon\alpha c_K$ and Q_0 have the same sign near these equilibrium points. Therefore, ϵ is not allowed to change its sign in the nearby configuration space.

Big bang and big rip solutions These fixed points correspond to $h^{\text{fp}} = 1$, i.e. $H^{\text{fp}} \rightarrow \infty$. Hence, the condition $(2\alpha - 1)\epsilon c_G > 0$ is necessary for the energy density (4.53) to be positive when the Hubble rate diverges. This constraint applies to E_3

and \mathcal{B}_3 in table 4.3. Consequently, ϵ cannot change its sign in the configuration space around these equilibrium points. Moreover, from comparing equations (4.14) and (4.52) it follows that $(2\alpha - 1)c_G$ and Q_0 should have the same sign. Therefore, the constant μ_3 appearing in equation (4.57) is well-defined and, in fact, positive.

Fixed Point	$\alpha < 0$	$0 < \alpha < \frac{1}{2}$	$\frac{1}{2} < \alpha < 1$
B_3 (vacuum)	$(c_K < 0)$	-	-
E_3 (BB/BR)	-	$(\epsilon c_G < 0)$	$(\epsilon c_G > 0)$
S_3^1 (dS)	$\{(c_K > 0, \epsilon c_G < 0), (c_K < 0, \epsilon c_G > 0)\}$	$(c_K < 0, \epsilon c_G < 0)$	$(c_K < 0, \epsilon c_G > 0)$
S_3^2 (dS)	-	$\{(c_K > 0, \epsilon c_G < 0), (c_K < 0, \epsilon c_G > 0)\}$	-
\mathcal{B}_3 (BB)	-	-	-

Fixed Point	$\alpha = 1$	$1 < \alpha$
B_3 (vacuum)	-	-
E_3 (BB/BR)	-	-
S_3^1 (dS)	$(c_K < 0, \epsilon c_G > 0)$	$(c_K < 0, \epsilon c_G > 0)$
S_3^2 (dS)	-	-
\mathcal{B}_3 (BB)	$(\epsilon c_G > 0)$	-

Table 4.4: Necessary constraints for the scalar field energy density (4.53) to be positive near the equilibrium points dominated by the scalar field. The conditions on c_K , c_G and ϵ are shown only when the corresponding fixed point acts as an attractor or a repeller in the configuration space, i.e. when trajectories in the configuration space undoubtedly approach or move away from that solution. Note that E_3 is not a fixed point when $\alpha = 1/4$ (see table 4.3). A set of conditions is showed in parenthesis. Multiple possible sets of conditions are grouped in curly brackets. Parameters that are not mentioned remain unrestricted. To enhance the readability of the table, the cases with $\alpha < 1$ are presented at the top of the page, while the remaining cases ($\alpha \geq 1$) are positioned just below.

De Sitter solutions These are the equilibrium points S_3^1 and S_3^2 in table 4.3. In order to constrain c_K , c_G and ϵ we impose $J = 0$ and $\varrho_\phi > 0$ in equations (4.52) and (4.53), respectively. The results (for an expanding FLRW) are shown in table 4.4. Note that we have limited our analysis to those values of the parameter α for

which the corresponding dS solutions act as attractors in the configuration space. This is to ensure that physical trajectories in the configuration space approach these solutions.

4.5 Conclusions of the chapter

The possibility of a stable self-tuning dS attractor in the shift-symmetric KGB theories has naturally attracted the attention of the scientific community [168, 199–203, 207]. Furthermore, revising the literature it could seem that this is the only possible future evolution for these cosmological models. Nevertheless, different future evolutions are indeed possible [2, 3]. In order to analyse this claim, we have proposed a dynamical system formulation never applied before to shift-symmetric KGB theories. The key feature of this new formulation is the compactification of the Hubble rate in the configuration space. This makes the configuration space truly compact which, in turn, allows for the proper identification of cosmological singularities where the Hubble rate and its cosmic time derivative diverge but the ratio \dot{H}/H^2 keeps bounded (i.e C_1 finite) as fixed points of the system. The physical interpretation of these cosmological singularities may vary depending on when and where they take place in the configuration space.

Owing to the structure of the dynamical equations (4.20)-(4.22), we have found five different groups of fixed points. The existence and stability of these fixed points, however, depends ultimately on the choice of the functions K and G of the system. In sections 4.3.1 to 4.4, we have applied this description to different power law examples. For these power law functions, different future cosmic singularities acting as attractors in the corresponding configuration space have been identified. Most notoriously, having a future evolution towards a BR singularity was found to be always possible for some values of the parameters in the proposed models. This is (to the best of our knowledge) the first time this cosmic singularity has been explicitly found in the shift-symmetric KGB sector. Thus, our findings advocate for a richer future phenomenology of the KGB theories than previously expected. Indeed, we consider this broader future phenomenology to significantly contribute to the interest of shift-symmetric KGB models in cosmology. Despite this success in our approach, it should be emphasised again that there may be equilibrium points that have eluded this classification because of the choice of the dynamical variables being not adequate for them to be correctly identified. Examples of potential interest for cosmology would be configurations corresponding to bounce or turnaround events.

In addition to the previous considerations, we have also identified the occurrence of BF and sudden singularities for the KGB model (4.39). To the best of our

knowledge, this is indeed the first time finite scale factor singularities are discussed in this context. Moreover, the presence of finite-size singularities also provides an excellent example of why $J = 0$ is not, as we argued at the beginning, an exhaustive characterization of all the possible future evolutions for an expanding universe in the shift-symmetric KGB theory. This is because the observable universe reaches a maximum size and, therefore, the shift-current (4.14) is non-trivial on the attractor as long as the shift-charge Q_0 is not null.

It should be highlighted, however, that the analysis of the background cosmic evolution we have performed here must be combined with a discussion on the stability of the cosmological perturbations in order to properly address the viability of the KGB models under consideration. The conditions for the absence of ghost and gradient instabilities for scalar perturbations were already obtained in references [40, 168] (see also references [194, 216]). Therefore, the fulfilment of these conditions at least at the vicinity of the fixed points obtained in tables 4.1 to 4.3 should be considered as a necessary but not sufficient condition for the stability of the scalar perturbations during the whole evolution. At the vicinity of the scalar field dominated fixed points with a phantom EOS (i.e. $w_\phi^{\text{fp}} + 1 < 0$) we have discussed in this chapter, which are the main results of our approach, the ghost and/or gradient condition are always violated. This may signal that the phantom solutions we have discussed are not viable from the point of view of the scalar perturbations. Nevertheless, it would be worthwhile to investigate the stability conditions not only at the vicinity of the fixed points here discussed but on the whole orbits, and for different (not only power law) KGB models. This will be the topic of the next chapter.

5 Stability of shift-symmetric scalar field theory

IN the previous chapter, we have discussed the possibility of modelling a DE component (at the background level) in the framework of scalar field theories. There we have focused on shift-symmetric scalar theories since this symmetry potentially avoids some of the fine-tuning problems that inevitably accompany the cosmological constant. We also restricted our attention to scalar theories satisfying that the propagation speed of GWs is equal to the speed of light. These considerations have led us to investigate shift-symmetric KGB theory, which is best-known for producing self-tuning dS future solutions [40]. Nevertheless, different future phenomenology can also be readily accommodated in this shift-symmetric framework [2, 3].

In this chapter, we analyse the stability of the shift-symmetric KGB theory against cosmological perturbations. First, we re-analyse the interrelation between phantom behaviour and classical and semi-classical instabilities of the scalar field in the framework of linear cosmological perturbations. By implementing a new characterization of the already-known stability conditions, we shed some light on previous results in the literature about the k -essence theory [160] (see also, for instance, references [96, 97, 176, 188, 439]) and also obtain new compact results for the braiding term.

Nevertheless, the absence of instabilities at linear order in scalar perturbations is a necessary but not a sufficient condition for the stability of the classical theory. Indeed, it has been shown that the interaction mediated by the *braiding* term between tensor perturbations (essentially GWs) and DE fluctuations may induce a ghost-like and/or gradient-like instability in the scalar sector [286]. (See also references [183, 440] for a discussion on the decay of GWs into scalar fluctuations when Lorentz invariance is spontaneously broken.) Consequently, it has been concluded that the braiding term in the KGB theory should not produce any sizeable effect in order to trivially escape from this GWs-induced instability [286]. According to these results, the available parameter-space of the shift-symmetric KGB models seems to shrink to that of the shift-symmetric k -essence theory only [286]. In the second part of this chapter, therefore, we reflect on the instability induced by this DE-GWs interaction. Analysing the assumptions behind the mentioned conclusion, we propose a possible way to circumvent this obstacle when departing from the Galileon terms for the KGB functions. Unfortunately, we shall argue that the apparent loophole seems to lack practical applicability for constructing viable

DE models with a non-vanishing braiding term. In order to perform this study, we have derived the detailed form of the mass parameters of the KGB theory in the EFT approach. Although the expressions for these parameters were already computed at leading order, to the best of our knowledge, this is the first time that the complete family of parameters up-to arbitrary order is presented.

The content of this chapter is based on the peer-reviewed publication [1]. The chapter is organised as follows: section 5.1 is entirely devoted to the stability of linear-order scalar perturbation in the shift-symmetric KGB theory. The stability of the well-known k -essence subclass of the more general KGB framework is reviewed in section 5.1.1. In sections 5.1.2 and 5.1.3 we discuss the stability of linearised scalar perturbation for the remaining part of the KGB theory. Section 5.2 is devoted to the interaction of the braiding term with GWs. We review the arguments presented in reference [286] in section 5.2.1. We identify a potential mechanism to ease the constraints found in reference [286] in section 5.2.2. In section 5.2.3, we discuss that the possibility for a viable KGB model to implement such a mechanism is an elusive ambition in practice. Therefore, in section 5.3, we reflect on the open paths that can still be further explored to find fundamental viable descriptions for DE. Finally, auxiliary results for discussing the stability of linear perturbations are summarised in appendix D. Useful calculations and a self-contained dictionary between the covariant version of the scalar field theory and that of the EFT approach are presented in appendix E.

5.1 Stability of linearised scalar perturbations

The stability of scalar perturbations around a flat FLRW background has already been addressed at linear order for the shift-symmetric KGB theory [40] (see also references [41, 168, 194]). The quadratic action describing scalar perturbations runs as follows [40, 168]

$$S_{\text{scalar}}^{(2)} = \int d^4x a^3 Q_S \left[\dot{\zeta}^2 - \frac{c_s^2}{a^2} (\partial_i \zeta)^2 \right], \quad (5.1)$$

where ζ represents the curvature perturbation as commonly defined (see, for example, reference [40]), Q_S is the normalization factor of the kinetic term, and c_s denotes the speed of sound of the scalar perturbation. From the above action, the absence of a ghost instability in the scalar sector demands [40, 194]

$$Q_S := \frac{2D}{(2 - \alpha_B)^2} > 0, \quad D := \alpha_K + \frac{3}{2}\alpha_B^2, \quad (5.2)$$

whereas the absence of a gradient instability implies [40, 194]

$$c_s^2 := -\frac{(2 - \alpha_B) \left[\dot{H} - \frac{1}{2} H^2 \alpha_B \right] - H \dot{\alpha}_B + \varrho_m + \frac{4}{3} \varrho_r}{H^2 D} \geq 0, \quad (5.3)$$

where the dimensionless functions α_K and α_B were first introduced in reference [194]. They are defined as

$$H^2 \alpha_K := 2X (K_X + 2X K_{XX}) + 12\dot{\phi} X H (G_X + X G_{XX}), \quad (5.4)$$

$$H \alpha_B := 2\dot{\phi} X G_X. \quad (5.5)$$

Please note that condition (5.2) trivially reduces to $D > 0$, since the denominator of Q_S is always positive. Violation of this condition leads to scalar perturbations whose associated kinetic energy takes negative values [190]; i.e. the perturbations become ghost-like. The presence of a ghost DOF may be detrimental (at the classical level) if the ghost interacts with a positive-energy mode, as this may lead to runaway solutions where the total energy is conserved but the relative energies associated to the ghost and no-ghost sectors diverge (see, for instance, reference [290]). At the quantum level, the corresponding ϕ -particles would have negative energies. In this case the vacuum becomes unstable due to the spontaneous production of ghost-particles together with normal-particles with arbitrarily high energies and momenta [290] (see also reference [190]). Consequently, backgrounds with ghosts are generally considered pathological at both classical and quantum regimes. On the other hand, violation of condition (5.3) introduces the so-called gradient instability. This is when the leading order spatial derivatives have the wrong sign w.r.t. the time derivatives in the perturbed action (5.1) (see also references [190, 287]). In Fourier space, the frequencies of the oscillations become imaginary at high momenta, resulting in perturbations that grow exponentially fast. Thus, it precludes a stable classical model (at least, as long as a perturbative treatment is still valid).

It is interesting to note that

$$H^2 D = 2X (A + 6X^2 G_X^2), \quad (5.6)$$

where A has been defined in expression (4.11). As a result, the ghost-free condition $D > 0$ (see equation (5.2)) implies

$$A + 6X^2 G_X^2 > 0, \quad (5.7)$$

in the notation of the previous chapter. Moreover, replacing the time derivative of the Hubble rate that appears in the scalar field equation (4.10) by means of the Raychaudhuri equation (4.4) leads to

$$H^2 D \ddot{\phi} + 6X J \left(H - \dot{\phi} X G_X \right) - 2X^2 G_X (4\varrho_r + 3\varrho_m) = 0. \quad (5.8)$$

Hence, the ghost parameter D is just the factor ahead of the scalar field acceleration once the derivatives of the metric DOF are removed from the scalar field equation (4.10). However, this is precisely the combination appearing in the denominator of the auxiliary functions C_1 and C_2 ; see appendix A. Thus, the problematic scenarios discussed in the previous chapter, where the denominator of these functions vanishes, actually correspond to the limit $D \rightarrow 0$ within the physical configuration space. Generally, this condition may signal the presence of a pressure singularity which the dynamics cannot penetrate [40, 194], as observed in the models explored in sections 4.3.2 and 4.4.

In the following we will analyse the stability conditions described in equations (5.2) and (5.3) for three different scenarios: (i) the k -essence model ($G \equiv 0$), (ii) a braiding model with $K \equiv 0$, and (iii) the most general KGB scenario. These are sections 5.1.1, 5.1.2 and 5.1.3, respectively. In doing so we will review some well-known facts and also face new discussions about the viability of these shift-symmetric theories from the point of view of linear cosmological perturbations.

5.1.1 k -essence

Let us first re-analyse the stability for the well-known k -essence case [96, 98, 176–178]. This corresponds to setting the braiding function G to zero in action (4.2), although a non-zero but constant braiding function would also reduce to the k -essence scenario. From this point of view, one may consider the k -essence theory as a special sub-case of the more general KGB action (4.2). However, it is worth noting that the two scalar field theories have very different properties. This is because second order derivatives of the metric and scalar field are no longer mixed when G is constant. Thus, some of the most interesting features of the KGB set-up (such as stable phantom crossing) are not present in the k -essence scenario. Still, k -essence represents the most general scalar theory whose action contains up-to first order derivatives of the scalar field and has been extensively explored in a wide variety of cosmological scenarios, from inflation [96, 97] to DE [98, 176–178].

Unlike the scalar field with a canonical kinetic term, for a k -essence field a phantom behaviour is not necessarily due to the presence of a ghost [188] (see also [160]), since equation (5.2) reduces to

$$Q_s = \frac{D}{2} = \frac{X}{H^2} \frac{d\varrho_\phi}{dX}, \quad (5.9)$$

whereas the violation of the NEC by the scalar field depends on the slope of the k -essence function K ,

$$1 + w_\phi = \frac{2XK_X}{\varrho_\phi}, \quad (5.10)$$

being

$$\varrho_\phi = 2XK_X - K, \quad (5.11)$$

$$p_\phi = K. \quad (5.12)$$

Compare with expressions (4.8) and (4.9) when G_X is trivial. The slope of the function K should be negative for a phantom field, but this does not necessarily force the energy density ϱ_ϕ to be a decreasing function of the kinetic term. So, the sign on the right-hand side of equation (5.9) is in principle independent of that of equation (5.10); see reference [188].

The relation between instabilities and phantom behaviour appears when considering the squared speed of sound of scalar perturbations, i.e. c_s^2 . Taking into account the Friedmann equation (4.4), we can recast the gradient-free condition (5.3) as [1] (see also [191])

$$c_s^2 = \frac{3(1+w_\phi)\Omega_\phi}{D} \geq 0, \quad (5.13)$$

where $\Omega_\phi = \varrho_\phi/3H^2$ is the partial energy density for the scalar field and we have also used the fact that $\alpha_B \equiv 0$ for k -essence. This new reformulation of the expression for c_s^2 is extremely useful since we can address the stability of linear perturbations in terms of background quantities for which we have a strong physical intuition. Focussing on the case $\Omega_\phi > 0$, this inequality shows an interrelation between the ghost-free and gradient-free conditions with the possible phantom character of the ϕ -fluid. In particular, if the NEC is satisfied for the scalar field (i.e. when $1+w_\phi > 0$), there is not a gradient instability if and only if the ghost-free condition is also satisfied. As a result, there are quintessence-like k -essence models with a completely stable scalar spectrum. On the other hand, the gradient-free and ghost-free conditions become anti-correlated when the NEC is violated at the level of the ϕ -fluid. That is to say, c_s^2 is positive for a phantom fluid only if a ghost-like instability is present and vice-versa, scalar perturbations are ghost-free only if a gradient instability is triggered. Please, note that the same conclusion was reached in reference [160], albeit through a different reasoning (see also references [188, 189]).

As is well-known, it is not possible to describe an effective phantom fluid via a scalar field *à la* k -essence in a way that both ghost and gradient instabilities are absent [160, 188–190]. However, let us reflect about the nature of these instabilities (see, for example, reference [190] for a review on the topic). On the one hand, the presence of a gradient instability is related to a wrong sign for the spatial derivatives in the perturbed action (5.1). This makes the frequencies of the fluctuations imaginary at high momenta, resulting in perturbations that grow arbitrarily fast. Thus, it precludes a stable classical model (at least, as long as a

perturbative treatment is still valid). For a ghost mode, on the other hand, the associated kinetic energy is negative. If the ghost DOF interacts with a positive energy mode (at the classical level) there may be runaway solutions, where the total energy is conserved while individual energies diverge; we refer the interested reader to the discussion in, for example, reference [290]. As a result, the common lore states that ghost instabilities are catastrophic (already) at classical level. Still, the classical background is stable against high momenta perturbations [190]. It is interesting to note that there are examples in the literature in which the presence of a ghost DOF interacting with a positive energy DOF does not lead to runaway solutions and, therefore, to the destabilization of the classical motion of the system [291]. (See also *islands of stability* [292, 293] and *meta-stability* of ghosts [294, 295].) Upon canonical quantisation of theories with ghosts, the energy conservation does not forbid pair creation from vacuum of ghosts-particles together with normal-particles: the vacuum becomes quantum mechanically unstable (see, for instance, references [190, 290]). So, the presence of a ghost is also considered to be pathological at the semi-classical level. However, the possibility of safely living with ghosts at the quantum level has already been explored with positive conclusions [296, 300, 303, 305] (see also references [306, 307] for applications to quadratic gravity). Therefore, even if it is clear that the presence of any of these instabilities (ghost and/or gradient) is a red light that has to be seriously taken into account, it would be interesting to consider the possibility that the scalar field (understood as being of gravitational nature) should be quantized in a different way to matter fields (for example, with the spacetime itself [297, 299]) or not being quantized at all, when dealing with the ghost instability. For a review on the topic see, for example, reference [48].

In this context, a gradient instability is hardly tameable in the classical theory, whereas a ghost-like instability could be further discussed at both classical and quantum regimes. So, if one considers that the H_0 tension has to be solved by means of a phantom fluid, then, our best hope in the k -essence case would be selecting the function K in such a way that only the ghost-free condition is violated. Otherwise, a negative c_s^2 will inevitably jeopardise the perturbative approximation due to fast growing fluctuations. In addition, it was shown in reference [191] (see also [192]) that the scalar field in the k -essence theory, whether shift-symmetric or not, cannot cross the phantom divide. Consequently, the EOS parameter for the scalar field, namely w_ϕ , remains always no greater than or no less than -1 for a single scalar field *à la* k -essence. Nevertheless, a phantom-crossing in the DE sector was analytically shown to be a prerequisite for solving both the H_0 and S_8 tensions simultaneously [131, 132]. (Similar conclusions were also reached by addressing the resolution of the H_0 tension only [175, 193].) Therefore, if both

tensions were considered on the same footing¹, a scalar field theory beyond k -essence should be explored. See also references [175, 193] for previous works on the H_0 tension.

5.1.2 Braiding model

We now analyse the case of $K \equiv 0$ in action (4.2). This is a straightforward limiting scenario of the complete KGB framework where the contribution of the k -essence part is negligible. However, contrary to pure k -essence discussed in the previous section, second order derivatives of the metric and scalar field are still mixed in the corresponding field equations due to the function G ; see equations (4.4) and (4.10). As a result, this is a simpler scenario than the complete KGB theory. Still, it provides us with an interesting candidate for addressing the stability properties of the *kinetic braiding*.

The expressions for the energy density and pressure of the scalar field in equations (4.8) and (4.9), respectively, simplify to

$$\varrho_\phi = 6\dot{\phi}XG_XH, \quad (5.14)$$

$$p_\phi = -2XG_X\ddot{\phi}, \quad (5.15)$$

where the expression for J in equation (4.7) has been also considered. Then, the EOS parameter for the scalar field reads

$$w_\phi = -\frac{\ddot{\phi}}{3\dot{\phi}H}. \quad (5.16)$$

The scalar field acceleration, $\ddot{\phi}$, can be removed from the previous expression by means of the Raychaudhuri equation (4.4) combined with the scalar field equation (4.10). Then, after simple manipulations we can re-write the scalar field EOS parameter as

$$w_\phi = \frac{\Omega_\phi(3 - \Omega_r)}{2D}, \quad (5.17)$$

where $\Omega_r = \varrho_r/3H^2$ is the partial energy density for radiation and the contribution of matter has been removed through the constraint (4.18). Please note that the

¹Note that the disagreement between the value of H_0 inferred from Planck-CMB [79] and that coming from the direct local distance ladder measurements provided by the SH0ES team [82, 441] has reached a statistical significance of more than 5σ . Whereas the S_8 tension is at much lower statistical significance, reaching between 1.7 to 3 standard deviations; see for instance [33] and references therein. We refer the interested reader to the review [35] for a self-contained discussion about the observational tensions in the standard cosmological model.

above expression allows us to re-express the ghost-free condition (5.2) in terms of background quantities only. This is

$$D = \frac{\Omega_\phi(3 - \Omega_r)}{2w_\phi} > 0. \quad (5.18)$$

As emphasised in the previous section, this new approach to the evaluation of the stability conditions is extremely useful since we have a strong physical intuition for the values of background quantities. The actual dependence of the EOS parameter on the geometry and the scalar field parameters, that is to say $w_\phi = w_\phi(a, \dot{a}, \dot{\phi}, \ddot{\phi})$, will depend on the choice for the braiding function G . However, if we assume a positive Ω_ϕ , it follows from the above inequality that a ghost instability is always present if w_ϕ is negative. A remarkable implication of this result is that any model of the form $G \square \phi$ that aims to describe a DE component (not necessarily phantom-like) will inevitably have this instability, since DE requires breaking the SEC at the level of the geometry. In other words, w_{eff} should be less than $-1/3$ and, therefore, $w_\phi < -1/3$ should hold as well.

A similar derivation can also be conducted with the expression for the speed of sound squared in expression (5.3). Straightforward differentiation over the definition for α_B in equation (5.5) leads to

$$\frac{\dot{\alpha}_B}{H} = 3(w_{\text{eff}} - w_\phi)\Omega_\phi, \quad (5.19)$$

where we recall that $w_{\text{eff}} = p_{\text{tot}}/\rho_{\text{tot}}$ represents the effective EOS parameter of the total fluid on the right-hand side of equations (4.3) and (4.4). Taking this result into account, and also substituting \dot{H} by means of equation (4.4), the gradient-free condition (5.3) can be re-formulated in terms of background densities as

$$c_s^2 = \frac{\Omega_\phi(5 - \Omega_\phi + 3w_{\text{eff}})}{2D} \geq 0. \quad (5.20)$$

The numerator in the above expression can be positive or negative depending on the values of Ω_ϕ and w_{eff} . In Figure 5.1, we represent the fulfilment of the stability conditions in the $(\Omega_\phi, w_{\text{eff}})$ -plane. As there can be checked, it is possible to have ghost-free and gradient-free scalar perturbations during radiation and matter dominated epoch; that would correspond to $w_{\text{eff}} \approx 1/3$ and $w_{\text{eff}} \approx 0$ for $\Omega_\phi \ll 1$, respectively. A necessary and sufficient condition for this to happen is that of w_ϕ being positive during that period; see inequality (5.18). On the contrary, perturbations will always become unstable at some point if w_ϕ is negative; for example, if the braiding scalar field acts as DE. Hence, an accelerating universe cannot be safely modelled when $K \equiv 0$ in the KGB action (4.2), as this would inevitably produce ghost and gradient unstable scalar perturbations. Interestingly,

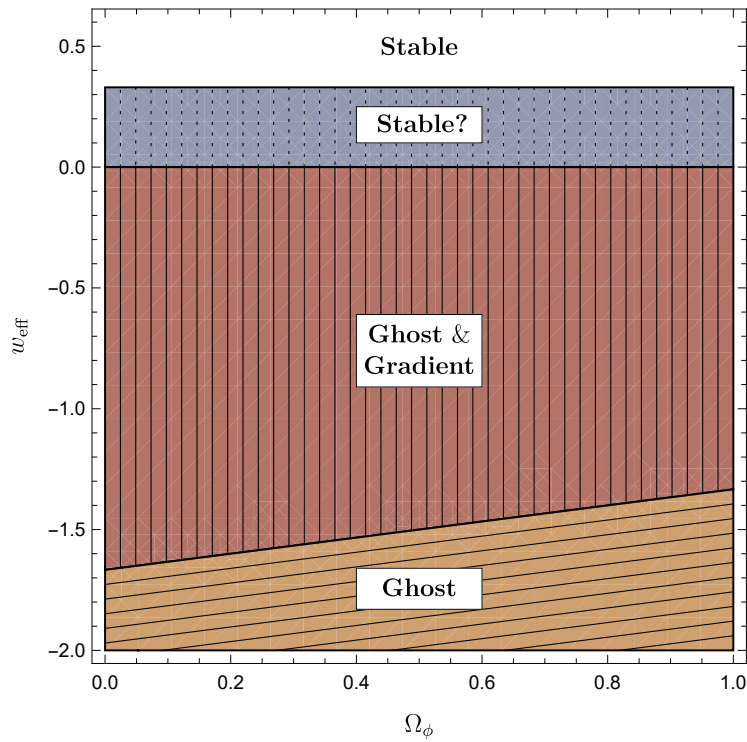


Figure 5.1: Stability of scalar perturbations in the $(\Omega_\phi, w_{\text{eff}})$ -plane for $K \equiv 0$. The lower oblique-lined region corresponds to the presence of a ghost instability. Scalar perturbations are both ghost- and gradient-unstable in the central vertical-lined region. Stability is ensured in the $w_{\text{eff}} > 1/3$ zone, since w_ϕ is clearly positive there in virtue of the relation $w_{\text{eff}} = \Omega_r/3 + w_\phi \Omega_\phi$. In the dotted region, which corresponds to the horizontal band $0 \leq w_{\text{eff}} \leq 1/3$, perturbations may be healthy if and only if w_ϕ is non-negative, otherwise they will be both ghost- and gradient-unstable. Nevertheless, the sign of w_ϕ in that region of the $(\Omega_\phi, w_{\text{eff}})$ -plane cannot be inferred without solving the whole evolution of the model and, therefore, the stability conditions there cannot be further addressed without specifying the function G .

c_s^2 could be positive for a super-accelerated regime ($w_{\text{eff}} < -1$), although this would only be possible at the price of having a ghost mode. This feature may be interesting for modelling phantom DE since, as we have discussed in the previous section, the positivity of the speed of sound squared can be argued to be more fundamental from a classical point of view than the absence of ghosts. However, from Figure 5.1 it is clearly not possible to have a braiding model (with $K \equiv 0$) that connects this gradient-stable super-accelerated (late-time) regime with a realistic early-universe description in a way that c_s^2 remains always positive during matter ($w_{\text{eff}} \approx 0$) and radiation ($w_{\text{eff}} \approx 1/3$) domination. Therefore, modelling DE with only the braiding part $G \square \phi$ of the KGB theory seems rather unwisely.

5.1.3 The complete KGB theory

In the previous sections we followed a novel approach to the evaluation of the stability of linear scalar perturbations by rewriting the ghost-free (5.2) and gradient-free (5.3) conditions in terms of background quantities, like the partial energy densities Ω_i and the EOS parameters w_ϕ and w_{eff} . Our main purpose with this approach is to have a better physical intuition about the requirements for a given model to produce stable scalar perturbations. From this analysis, we found that instabilities are always triggered when $1 + w_\phi < 0$ (violation of the NEC in the DE sector) in the case of k -essence. Moreover, modelling *kinetic braiding* only with the function G surprisingly makes things even worse, since now instabilities appear as w_ϕ becomes negative. Thus, no stable DE component (for which w_ϕ should be less than $-1/3$) can be produced in the case of $K \equiv 0$. In this section, we will apply the very same analysis to the full KGB theory.

When both K and G functions are non-trivial, the ghost-free condition (5.2) cannot be directly re-expressed in terms of the previous background quantities. However, it is possible to write

$$D = \frac{3\Omega_J^B [3\Omega_J(\Omega_J^B - 2) + (3 + \Omega_r - 3\Omega_\phi)\Omega_J^B]}{6[\Omega_J - (1 + w_\phi)\Omega_\phi]} > 0, \quad (5.21)$$

where

$$\Omega_J := \frac{\dot{\phi}J}{3H^2}, \quad (5.22)$$

$$\Omega_J^B := \frac{2\dot{\phi}XG_X}{H}, \quad (5.23)$$

are the partial energy densities for the contributions of the shift-current, J , and that of the braiding function, G , to the different terms in the expression for scalar field energy density ϱ_ϕ in equation (4.8), respectively. Please note that Ω_J^B coincides with the definition of α_B [194], see equation (5.5). It is also important to highlight that the physical constraint of $\Omega_\phi \in [0, 1]$ does not imply, in general, any bound on the value of these auxiliary partial energy densities. Their value can be arbitrary large and/or negative.

Similarly, the gradient-free condition (5.3) can be translated to

$$c_s^2 = \frac{1}{D} \left\{ \frac{\Omega_J^B(2 - \Omega_J^B)}{2} + 3\Omega_J + 3(2 + \eta)[\Omega_J - (1 + w_\phi)\Omega_\phi] \right\} \geq 0, \quad (5.24)$$

being

$$\eta := \frac{2XG_{XX}}{G_X}, \quad (5.25)$$

a relevant quantity for the discussion in the next section. Please note that when G or K are trivial, the above expressions reduce to those obtained in sections 5.1.1 and 5.1.2, respectively.

Contrary to the limiting cases analysed in the previous sections, conditions (5.21) and (5.24) can be satisfied simultaneously for a wide variety of models including those with phantom behaviour. For instance, assuming η to be positive (as this will be crucial in the forthcoming sections), we present all possible cases where both inequalities are satisfied in appendix D. Nevertheless, since Ω_J^B and Ω_J are not physically meaningful quantities as Ω_ϕ is, it is difficult to extract the most general conditions the functions K and G should meet in order to produce a stable model. Anyway, examples of such models can be easily constructed; see, e.g., figures 5.3 and 5.5 in the next sections. More examples can also be found in the literature. For example, in reference [40] the authors analyse the case of K and G being proportional to X . They also show there that the resulting cosmological model has completely stable linear scalar perturbations even though the scalar field is violating the NEC. (Note, however, that their model does not feature super-acceleration since $1 + w_{\text{eff}} > 0$ always.) See also references [168, 346, 435, 436] for more examples of stable KGB models. Hence, it is possible to construct reliable cosmological models with the scalar field coming from shift-symmetric KGB theories when both k -essence and braiding functions are non-trivial.

5.1.4 Summary

Could we describe a stable DE component with a scalar field coming from shift-symmetric KGB theories? There is no problem to describe DE with a k -essence term if the scalar field satisfies the NEC. That is a quintessence-ish scalar field theory involving only up-to first order derivatives of ϕ . However, it is well-known that k -essence suffers from instabilities if the scalar field violates the NEC [160, 188–190]. Moreover, the scalar field energy density should be always phantom or non-phantom since k -essence cannot produce a phantom-crossing [191] (see also [192]). Hence, if we interpret current data as favouring the presence of a slight violation of the NEC in the DE sector at present times, then, the scalar field should have always violated the NEC. In this scenario, a k -essence proposal will be plagued with a gradient or a ghost instability. With an appropriate selection for the function K , however, the gradient-free condition can be satisfied, in principle, even for NEC-violating models. Nevertheless, the resulting scalar field will feature a ghost DOF; yet this may not always be as catastrophic as commonly stated. As we have discussed, it would be interesting to explore whether it is possible to have a ghost mode in cosmology without destabilising the classical nor the semi-classical regimes of the theory. While this may be feasible, addressing both the

H_0 and S_8 tensions (in case the latter is still present in future surveys) by means of late-time physics only continues to pose an insurmountable obstacle in the k -essence scenario, since no phantom-crossing is possible (see discussion in references [131, 132]). Indeed, focusing on the H_0 value only, k -essence has been argued to make the tension even worse [175, 193].

The situation is significantly worsened when only the braiding function G is present in the scalar field's action (4.2). Scalar perturbations are always ghostly if the scalar field acts as a DE component, which demands $w_\phi < -1/3$ (see condition (5.18)). This is aggravated even further by the fact that a gradient instability is also present in any realistic model that interpolates between an initial radiation dominated epoch ($w_{\text{eff}} \approx 1/3$) and a late-time accelerated expansion regime ($w_{\text{eff}} < -1/3$); see Figure 5.1. Hence, the term $G\Box\phi$ alone in the shift-symmetric action (4.2) is not a viable option for modelling DE.

Finally, when considering the sum of k -essence and the braiding term the situation is different. Following the same strategy we have used to analyse the preceding marginal examples, we have recovered the well-known result that the conditions for the avoidance of ghost and gradient instabilities can be simultaneously fulfilled even when the ϕ -fluid violates the NEC (see appendix D). Although the lack of a physical intuition for the auxiliary quantities Ω_J and Ω_J^B did not allow us to restrict the possible phenomenology of the theory as stringently as for the previous cases, note that linearly stable KGB models have been already reported in the literature (see for instance [168, 346, 435, 436] and references therein). This fact points to the viability (from the point of view of the stability of linear scalar perturbations) of modelling a realistic DE component with the scalar field from the (complete) shift-symmetric KGB theory, at least in principle.

5.2 Beyond scalar perturbations

In section 5.1 we have discussed the absence of ghost and gradient instabilities in the linearised scalar perturbations around a flat FLRW background. In that approach, interactions between scalar, vector and tensor perturbations were not present, since they decoupled at the linear level. However, these interactions can emerge beyond the linear regime and may prove significant. In fact, the interaction between tensor perturbations (essentially GWs) and DE fluctuations may induce ghost and/or gradient instabilities in the scalar sector, as it was pointed out in reference [286]. In that case, the stability conditions discussed in the previous sections do not guarantee the viability of the theory², since the braiding term

²See also references [183, 440] for a discussion on the decay of GWs into scalar fluctuations when Lorentz invariance is spontaneously broken.

in the action can destabilize the theory through the GWs-DE interaction. As a concrete example, for cubic Galileon (which corresponds to $G(X) \propto X$) this effect is detrimental when $|\alpha_B| \geq 10^{-2}$; in other words, if the effects of the braiding are significant [286].

In general, the result of reference [286] raises serious doubts about the viability of any KGB theory (different from k -essence) aiming to describe the currently observed abundance of DE in the Universe. Nevertheless, as the authors of that reference commented (see also reference [442]), it is also important to analyse the fate of the instabilities once they are originated. The fate of the theory after the instability is reached is, however, uncertain since it depends on an unknown UV-completion.

In the following, we review the arguments and notation presented in reference [286]; that is section 5.2.1. In section 5.2.2 we obtain the general conditions a KGB model should meet in order to not be destabilised when interacting with GWs, even when the contribution from the braiding is non-negligible. The latter possibility turns to be attainable only if the braiding function G is not linear in the kinetic term X (i.e. if it is different from that of cubic Galileon). In section 5.2.3 we explore whether these conditions could be satisfied by some reasonable KGB model.

5.2.1 Interaction with gravitational waves: a review

In reference [286] the authors used the EFT approach to discuss the interaction between DE perturbations and GWs. (See appendix E for a review on the EFT approach to DE.) For this effect to manifest one needs a cubic coupling $\pi\pi\gamma$ in the perturbed action, where γ stands for tensor perturbations (essentially GWs) and π denotes scalar field fluctuations [286] (not to be confused with the scalar field ϕ itself). In the covariant version of the theory, the interaction $\pi\pi\gamma$ is related to the Cubic Horndeski operator; i.e. to the braiding term $G\Box\phi$ in action (2.21). Nevertheless, this interaction vertex is also present in beyond Horndeski theories [183, 286, 440].

The interaction between DE perturbations and GWs is conveniently addressed in the Newtonian gauge [286]

$$g_{00} = -(1 + 2\Phi) \quad \text{and} \quad g_{ij} = a^2(1 - 2\Psi)(e^\gamma)_{ij}, \quad (5.26)$$

where Φ and Ψ are the Newtonian potentials, and γ_{ij} is transverse and traceless. At leading order, the Lagrangian density describing this interaction reads [286]

$$\mathcal{L}_\pi = \frac{1}{2} [\dot{\pi}^2 - c_s^2 \partial_i \pi \partial^i \pi] + \mathcal{L}_{\text{int.}}, \quad (5.27)$$

being

$$\mathcal{L}_{\text{int.}} = -\frac{1}{\Lambda_{\text{B}}^3} \square \pi \partial_\mu \pi \partial^\mu \pi + \frac{\eta}{\Lambda_{\text{B}}^3} \ddot{\pi} \partial_i \pi \partial^i \pi + \Gamma^{\mu\nu} \partial_\mu \pi \partial_\nu \pi - \frac{\Lambda_{\text{B}}^3}{2} \pi \Gamma_{\mu\nu} \Gamma^{\mu\nu}, \quad (5.28)$$

where the time and spatial derivatives have been considered much larger than the Hubble rate [183, 286, 440] (see appendix E). Consequently, indices are raised/lowered with the Minkowski metric in the above expression. In addition, c_s^2 is given by expression (5.3) and

$$\Gamma_{\mu\nu} := \frac{\dot{\gamma}_{\mu\nu}}{\Lambda^2}, \quad (5.29)$$

$$\Lambda^2 := \frac{\sqrt{2} H^2 D}{\bar{m}_1^3}, \quad (5.30)$$

$$\Lambda_{\text{B}}^3 := -\frac{2H^3 D^{\frac{3}{2}}}{\bar{m}_1^3}, \quad (5.31)$$

being D the ghost factor (5.2). Moreover, the parameter η is defined through the relation [286]

$$4\bar{m}_2^3 = -(1 + \eta)\bar{m}_1^3, \quad (5.32)$$

where \bar{m}_1^3 and \bar{m}_2^3 are functions on the background time, t , that appears in the EFT action of the KGB theory; see expression (E.4). This parameter is useful for measuring deviations with respect to cubic Galileon (i.e. $G(X) \propto X$) for which η is identically zero and, therefore, $4\bar{m}_2^3 = -\bar{m}_1^3$. The covariant version of this parameter can be obtained from the expression for the mass parameters \bar{m}_1^3 and \bar{m}_2^3 in terms of the KGB functions and its derivatives (please, find further details in appendix E). Taking the expressions (E.41) and (E.42) into account, it is straightforward to obtain that the covariant version of η is nothing but the quantity we already have defined in equation (5.25). That is $\eta = 2XG_{XX}/G_X$.

The field equation for the scalar field perturbation, π , follows from varying the action corresponding to the Lagrangian density (5.27). This reads [286]

$$\begin{aligned} \ddot{\pi} - c_s^2 \nabla^2 \pi + \frac{2}{\Lambda_{\text{B}}^3} \left[(\partial_\mu \partial_\nu \pi)(\partial^\mu \partial^\nu \pi) - (\square \pi)^2 \right] + \frac{1}{2} \Lambda_{\text{B}}^3 \Gamma_{\mu\nu} \Gamma^{\mu\nu} + 2\Gamma^{\mu\nu} \partial_\mu \pi \partial_\nu \pi \\ + \frac{2\eta}{\Lambda_{\text{B}}^3} [(\partial_i \dot{\pi})(\partial^i \dot{\pi}) - \ddot{\pi} \nabla^2 \pi] = 0, \end{aligned} \quad (5.33)$$

where $\nabla^2 \equiv \eta^{ij} \partial_i \partial_j$. Here we will restrict our discussion to the case where π propagates in a subluminal way, that is when $c_s^2 < 1$ [286]. (The luminal and superluminal cases are discussed in reference [286].) In this scenario, the lightcone

for π is narrower than the one for the GWs, since $c_{\text{GWs}}^2 = 1$ [286, 440]. Consequently, DE fluctuations are not sensitive to the source of the GWs, provided we are far enough from the source of emission [286, 440]. To address the DE-GWs interaction, therefore, we can consider the following classical GW solution with linear polarization “+” travelling in the z direction [286, 440]

$$\gamma_{ij} = h_0^+ \sin[\omega(t - z)] \epsilon_{ij}^+, \quad (5.34)$$

being $\epsilon_{ij}^+ = \text{diag}(1, -1, 0)$ and h_0^+ the dimensionless strain amplitude. Then, it follows from the definition (5.29) that [286]

$$\Gamma_{00} = \Gamma_{0i} = 0, \quad \Gamma_{ij} = \frac{\beta c_s^2}{2} \cos[\omega(t - z)] \epsilon_{ij}^+, \quad (5.35)$$

being

$$\beta := \frac{2\omega h_0^+}{c_s^2 |\Lambda^2|} = \frac{\sqrt{2}\omega h_0^+}{H^2 c_s^2} \left| \frac{\bar{m}_1^3}{D} \right|, \quad (5.36)$$

a parameter³.

The field equation (5.33) simplifies significantly when written in the null coordinates [286]

$$u := t - z \quad \text{and} \quad v := t + z. \quad (5.37)$$

Since there is no intersection between the region where the source of emission of the GWs is active and the past lightcone of π (provided we are sufficiently far from the source of emission), there is a translational invariance along the v null coordinate [286]. This suggests the ansatz $\pi = \pi(u)$ for the solutions of the field equation (5.33). By defining

$$\varphi := \frac{\pi}{\Lambda_{\text{B}}^3}, \quad (5.38)$$

equation (5.33) reduces to [286]

$$\varphi''(u) = -\frac{\Gamma_{\mu\nu}\Gamma^{\mu\nu}}{2(1 - c_s^2)} = -\frac{\beta^2 c_s^4}{4(1 - c_s^2)} \cos^2(\omega u), \quad (5.39)$$

where prime denotes derivation w.r.t. the null coordinate u . In addition, the relations (5.35) have been used in the second equality. From the above expression it follows that φ is always decelerating along the null direction u .

³In this section we are closely following the notation used in reference [286]. Please do not confuse this parameter β with the exponent in the power law model (4.39) discussed in chapter 4.

The stability of a general solution to the equation (5.39), namely $\hat{\pi}$, can be addressed by analysing the tensor structure of the kinetic part related to the quadratic action for small fluctuations around that solution. That is, by considering $\pi = \hat{\pi} + \delta\pi$ and expanding the Lagrangian density (5.27) around the background solution $\hat{\pi}$ coming from equation (5.39). Taking into account only the kinetic terms for the fluctuation $\delta\pi$, this procedure leads to [286] (see also reference [285])

$$\mathcal{L}_{\text{kinetic}}^{(2)} = Z^{\mu\nu}(\hat{\pi}) \partial_\mu \delta\pi \partial_\nu \delta\pi, \quad (5.40)$$

where the values of the kinetic matrix $Z^{\mu\nu}$ depend on the spacetime coordinates through the background solution $\hat{\pi}$. These are [286]

$$Z^{00} = \frac{1}{2} + (2 + \eta)\varphi''(u) = \frac{1}{2} \left[1 - \frac{c_s^4 \beta^2}{2(1 - c_s^2)} (2 + \eta) \cos^2(\omega u) \right], \quad (5.41a)$$

$$Z^{11} = -\frac{c_s^2}{2} + \Gamma^{11} + \eta\varphi''(u) = -\frac{c_s^2}{2} \left[1 - \beta \cos(\omega u) + \frac{c_s^2 \beta^2}{2(1 - c_s^2)} \eta \cos^2(\omega u) \right], \quad (5.41b)$$

$$Z^{22} = -\frac{c_s^2}{2} + \Gamma^{22} + \eta\varphi''(u) = -\frac{c_s^2}{2} \left[1 + \beta \cos(\omega u) + \frac{c_s^2 \beta^2}{2(1 - c_s^2)} \eta \cos^2(\omega u) \right], \quad (5.41c)$$

$$Z^{33} = -\frac{c_s^2}{2} + (2 + \eta)\varphi''(u) = -\frac{c_s^2}{2} \left[1 + \frac{c_s^2 \beta^4}{2(1 - c_s^2)} (2 + \eta) \cos^2(\omega u) \right], \quad (5.41d)$$

$$Z^{03} = Z^{30} = (2 + \eta)\varphi''(u) = -\frac{c_s^4 \beta^2}{4(1 - c_s^2)} (2 + \eta) \cos^2(\omega u), \quad (5.41e)$$

where φ'' is given by equation (5.39). Let us recall again that we are considering here only the case of subluminal propagation for $\hat{\pi}$, i.e. $c_s^2 < 1$. See reference [286] for a discussion when $c_s^2 \geq 1$.

It should be highlighted that for a general time-dependent kinetic term like (5.40) there is no clear definition of stability [285]. However, in the limit where the time and length scales considered are much shorter than the rate of variation of $\hat{\pi}$, it is perfectly acceptable to analyse the stability of the system as if the kinetic matrix $Z^{\mu\nu}$ were constant [285] (see also reference [286]). Within this *local* approximation to the stability of the theory, the absence of a gradient instability can be determined as usual by analysing the relative signs between the terms involving time and spatial derivatives in the Lagrangian density (5.40). However, since the time and z direction are now mixed, it is convenient to move to Fourier space and directly study the dispersion relation for a mode with four-momentum $k^\mu = (\omega, k^i)$. For the Lagrangian density (5.40), the dispersion relation reads [285]

$$Z^{\mu\nu} k_\mu k_\nu = 0. \quad (5.42)$$

Multiplying this relation by Z^{00} , it is possible to re-express it as [285]

$$(Z^{0i}k_i - Z^{00}\omega)^2 = (Z^{0i}Z^{0j} - Z^{00}Z^{ij})k_ik_j, \quad (5.43)$$

when Z^{00} is not trivial. We recall that indices have been raised/lowered with the Minkowski metric. The absence of a gradient instability demands all frequencies, ω , to be real for any wave vector k^i . Otherwise, exponentially growing modes will be present. It is straightforward to notice from the above expression that this stability is guaranteed if the spatial matrix $Z^{0i}Z^{0j} - Z^{00}Z^{ij}$ is positive defined [285]. Since this matrix is diagonal for the $Z^{\mu\nu}$ introduced in equations (5.41), in our case of interest the positive-definedness condition simply reduces to

$$Z^{0i}Z^{0j} - Z^{00}Z^{ij} \geq 0, \quad (5.44)$$

for all spatial directions.

In addition to the previous condition, the ghost-like instability is avoided if [285]

$$Z^{00} > 0. \quad (5.45)$$

Please note that conditions (5.44) and (5.45) reduce to the standard ones when the matrix $Z^{\mu\nu}$ is in diagonal form [190].

When η is always trivial (that is when considering the case of cubic Galileon only, i.e. $G \propto X$), the ghost-free condition (5.45) leads to

$$|\beta| < \frac{1}{c_s^2} \sqrt{1 - c_s^2}, \quad (5.46)$$

which follows from demanding the factor ahead of the trigonometric term in equation (5.41a) to be less than one. Moreover, the expression $(Z^{03})^2 - Z^{00}Z^{33}$ is always positive when $\eta \equiv 0$. Therefore, there is not a gradient instability in the z direction. The background solution $\hat{\pi}$, on the other hand, does not affect the entries Z^{11} and Z^{22} . For $|\beta| > 1$, these entries oscillate between positive and negative values in a way that condition (5.44) could never be fulfilled. Avoiding this oscillations in the (x, y) -plane demands

$$|\beta| < 1. \quad (5.47)$$

For a non-relativistic speed of sound, that is $c_s \ll 1$, condition (5.47) is clearly more restrictive than the ghost-free condition (5.46). Therefore, by demanding $|\beta| < 1$ the stability conditions (5.44) and (5.45) are simultaneously fulfilled in the non-relativistic regime.

The complete stability region (including relativistic c_s) is shown in green in figure 5.2. As there can be seen, $|\beta| < 1$ is a necessary condition for the absence of ghost and gradient instabilities when η is trivial⁴. Owing to the definition of β in equation (5.36), this condition results in a tight constraint over \bar{m}_1^3 [286]. Please, note that there is a direct relation between \bar{m}_1^3 and α_B , which essentially measures the amount of *braiding* in the theory. This is

$$\bar{m}_1^3 = \alpha_B, \quad (5.48)$$

as follows from comparing equations (5.5) and (E.41). The observational bounds for α_B coming from the stability condition of $|\beta| < 1$ are discussed in reference [286]. To that aim, the authors there have considered a GWs-background as that generated by the event GW150914 [443] with a chirp mass of $M_c = 28M_\odot$ and $f = 30$ Hz at a distance of 1 Mpc. They found that the condition of $|\beta| < 1$ directly translates to $|\alpha_B| \leq 10^{-2}$ for that event [286], see the definition of β in equation (5.36). Thus, they conclude that the braiding part should not have any sizeable effect in order to avoid the destabilising interaction with GWs when η is zero [286]. Similar conclusions apply also to the case of $c_s = 1$ [286]. For the superluminal case, $c_s > 1$, it has been argued that the same results should hold as well, but no explicit calculations were provided due to technical difficulties [286].

On the contrary, if $\eta \neq 0$, then, oscillations in the spatial entries Z^{11} and Z^{22} can be avoided even for $|\beta| > 1$ provided that η is *sufficiently* large and positive. Hence, this may provide a mechanism for having a stable theory with $|\beta| > 1$. This was briefly commented in reference [286] but immediately discarded since the larger the value of η , the harder avoiding a ghost instability will be since this quantity enters linearly in the factor ahead of the trigonometric term in expression (5.41a). However, we find this conclusion to be premature as one should carefully explore the region of viability for the optimal effect when $\eta > 0$. If that is the case, then, the strong observational bounds for α_B discussed in reference [286] should be revised. We address this discussion in the next sections.

5.2.2 Loophole hunting

Condition (5.47) places a strong restriction to the maximum amount of *braiding* a theory may have in order to avoid the destabilising interaction with GWs described in reference [286]. As a result of that constraint, the braiding part should not have any sizeable effects when data from GWs events are taken into account [286]. However, this restriction holds only for the special case of $\eta \equiv 0$. In a more general situation, it would be possible to ease the constraint in equation (5.47) provided

⁴Note, however, that this conditions is not sufficient to guarantee the stability for values of c_s close to the speed of light.

that η is positive enough to ensure that all spatial directions in the kinetic matrix $Z^{\mu\nu}$ are negative. This is obviously not the case for $G \propto X$ for which η is trivial [286], but may be possible for models beyond a linear function G .

Inspired by the fact that the ghost-free condition (5.46) is less restrictive than the constraint in equation (5.47) for non-relativistic sound velocities when η is trivial, we explore here the possibility of a ghost-free and gradient-free theory with $|\beta| > 1$ when $\eta \neq 0$; recall the definition of β in equation (5.36). If that possibility comes to be true, then, the previously mentioned observational bound of $|\alpha_B| \leq 10^{-2}$ [286] should be revised. This may indicate that KGB theory could have sizeable effects at cosmological scales after all.

In general, the ghost-free condition (5.45) implies

$$|\beta| < \frac{1}{c_s^2} \sqrt{\frac{2(1-c_s^2)}{2+\eta}}, \quad (5.49)$$

which follows from demanding the factor ahead of the trigonometric term in equation (5.41a) to be less than one. The gradient-free condition (5.44) is automatically satisfied in the z direction since the combination

$$(Z^{03})^2 - Z^{00}Z^{33} = \frac{c_s^2}{4} \left[1 + \frac{(2+\eta)\beta^2 c_s^2}{2} \cos^2(\omega u) \right], \quad (5.50)$$

is always positive for the values of interest for η . Whereas in the (x, y) -plane the absence of a gradient instability implies

$$Z^{00}Z^{11} < 0, \quad (5.51)$$

$$Z^{00}Z^{22} < 0, \quad (5.52)$$

as follows from comparing the gradient-free condition (5.44) with the expressions for the $Z^{\mu\nu}$ found in equations (5.41). Contrary to the case of $\eta \equiv 0$, the oscillations in the spatial entries Z^{11} and Z^{22} can be avoided even for $|\beta| > 1$ provided that η is *sufficiently* large and positive. Taking into account their explicit expressions in equations (5.41b) and (5.41c), respectively, we found that for

$$\eta > \frac{1-c_s^2}{2c_s^2}, \quad (5.53)$$

these terms are always negative. Hence, a model satisfying the above condition will feature positive entries Z^{11} and Z^{22} . Consequently, it will be free from gradient instabilities in the (x, y) -plane provided that Z^{00} is positive. That is to say, if the ghost-free condition (5.49) is also satisfied. In other words, condition (5.49) and the new constraint found in equation (5.53) ensure the total stability of the system.

We should emphasise the fact that condition (5.53) does not depend on the specific properties of the GWs (local properties) but only on the value of c_s^2 , which depends on the KGB functions. It is also interesting to note that if scalar perturbations propagate close to the speed of light, then, condition (5.53) is easily satisfied if η is just slightly positive. However, this regime would strongly constrain β to vanish as follows from the ghost-free condition in equation (5.49). For a model with a non-negligible amount of braiding, this suggests that avoiding GWs-induced instabilities becomes more difficult if DE fluctuations propagate with a relativistic speed of sound. Conversely, the ghost-free condition (5.49) is compatible with $|\beta| \gg 1$ if c_s^2 is small. Nevertheless, η should diverge strongly than $1/c_s^2$ in order to avoid the gradient instability in this regime. This behaviour is summarised in figure 5.2. There we show different slices at constant η of the stability region where conditions (5.49) and (5.53) are simultaneously fulfilled. The green region corresponds to the case of $\eta \equiv 0$ (compare with figure 2 in reference [286]). As discussed before, the absolute value of β is always confined there to be less than one. Alternatively, this region becomes significantly bigger for small speed of sound if η is positive. In fact, stability at $|\beta| \approx 10$ is possible for η of the order of twenty. Please note that this supposes an enlargement of the stability region by a factor of ten w.r.t. the green zone. Moreover, this region can be amplified even more at low c_s for larger values of η . In the high c_s regime, however, the stability zone narrows compared to the case of η trivial.

In view of these results, we postulate that the would-be KGB candidate that could ease (to some extent) the restrictions from the interaction with GWs described in reference [286] must meet the following necessary (but not sufficient) conditions:

- It should produce a non-relativistic speed of sound, c_s , and a large value of η during the expansion history where interactions with GWs are expected.
- If DE perturbations propagate at relativistic speeds for the selected model, then, smaller values of η are preferred. Even so, the contribution of the braiding part should be negligible during the expansion history where interactions with GWs are expected.

The definition of c_s and η in terms of the KGB functions and its derivatives can be found in equations (5.3) and (5.25), respectively.

It should also be mentioned that, within the spirit of the discussion in past sections, one may consider the possibility to relax the ghost-free condition (5.49) and be concerned only with ensuring a gradient-free spectrum. Of course, this will drastically reduce the restrictions on the theory. Although the possibility of a ghost-mode in cosmology presents an interesting discussion, here there is

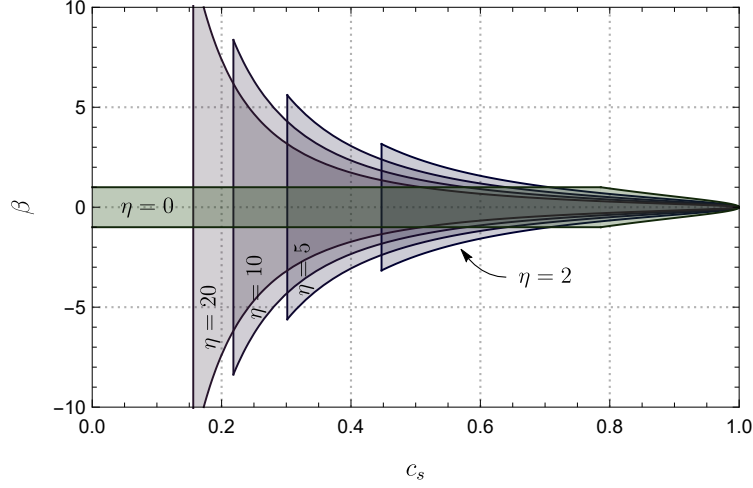


Figure 5.2: Slices at constant η of the stability region where conditions (5.49) and (5.53) are simultaneously satisfied. Within these regions, the interaction between DE fluctuations and GWs described in reference [286] does not induced a ghost nor a gradient instability. The green zone represent the stability at $\eta = 0$. This is the corresponding region for cubic Galileon, i.e. $G \propto X$ (compare with figure 2 in reference [286]). The darker shaded areas represent the stability at different non-zero values of η .

a technical difficulty in pursuing that direction. Given the structure of Z^{00} in equation (5.41a), if the condition (5.49) is violated then the sign of Z^{00} is not always negative (ghost mode excited) but fluctuates. Moreover, this fluctuation will jeopardise the relations (5.51) and (5.52) since the functional dependence of Z^{00} , Z^{11} and Z^{22} on $\cos(\omega u)$ is different. Thus, if the ghost-free condition is violated, then, gradient instabilities in the (x, y) -plane will also (periodically) appear within each fluctuation of the GWs. Consequently, relaxing the ghost-free condition is not a viable option here.

5.2.3 No natural dark energy

A natural shift-symmetric KGB candidate to test our hypothesis is that when η is a constant. From its expression in terms of G and its derivatives (5.25), this implies that

$$G(X) = c_G X^{\frac{2+\eta}{2}}, \quad (5.54)$$

being c_G a coupling constant. That is a power-law prescription for the braiding function G . Consequently, the case of η constant provides not only a natural choice to test our proposal but a physically relevant model. For this model, the resulting

speed of sound squared should be constrained as

$$\frac{1}{1+2\eta} < c_s^2 < 1, \quad (5.55)$$

in order to fulfil condition (5.53). This results in a lower limit for c_s^2 that should be satisfied (at least) during the cosmological evolution where interactions with GWs are expected. Please note that this is in agreement with the results previously presented in reference [444], where the possibility of a vanishing speed of sound was shown to be disfavoured. It should also be highlighted that, even though having a constant η is a very restrictive consideration, the results from exploring this case should also hold (at least asymptotically) for any other model for which η converges to a constant value. In other words, the physical conclusions from exploring a model like (5.54) should also apply asymptotically to any KGB theory for which the function G converges, at some point, to a power-law function.

In order to explore whether this mechanism can be conducted by a reasonable KGB model, we select a power-law function for the k -essence part as well. That is, we also consider

$$K(X) = c_K X^\alpha, \quad (5.56)$$

where α is a constant and c_K equals to $+1$ or -1 . For the KGB model given by the functions (5.54) and (5.56), we have numerically explored the parameter-space spanned by $\{(\eta > 0) \times \alpha \times c_G\}$. As our main purpose, at this stage, is to examine the stability of the KGB theory, not to confront it with observational data, we have considered the initial conditions $H_0 = 73.2 \text{ km s}^{-1} \text{ Mpc}^{-1}$, $\Omega_\phi^{(0)} \approx 0.68$, $\Omega_m^{(0)} \approx 0.32$ and $\Omega_r^{(0)} \approx 10^{-5}$, in line with local direct measurements as those reported in reference [82], at face value for the numerical integrations.

Our numerical analysis has shown two main tendencies for these models. First, we found that the ghost-free and gradient-free conditions discussed in section 5.1 (where scalar perturbations decouple from GWs at linear order) are not fulfilled for all the parameter-space, but only in some regions. Second, for the models that satisfy the ghost-free and gradient-free at linear order, we have found that the condition (5.53) is always violated at some point during the (past) evolution of the system. We summarise these findings with the two proxy KGB candidates shown in figures 5.3 to 5.7. In the former, we consider $\eta = 0.4$, $\alpha = 0.6$, $c_K = -1$ and c_G ranging from $9 \cdot 10^{-11}$ to $9.3 \cdot 10^{-11}$. As can be appreciated in figure 5.3, this simple KGB model has a compelling behaviour on the background level. Depending on the value of the coupling constant c_G , the fractional contribution of the scalar field to the total energy of the universe peaks at matter-radiation equality, rendering this model as a potentially interesting Early Dark Energy (EDE) candidate (see

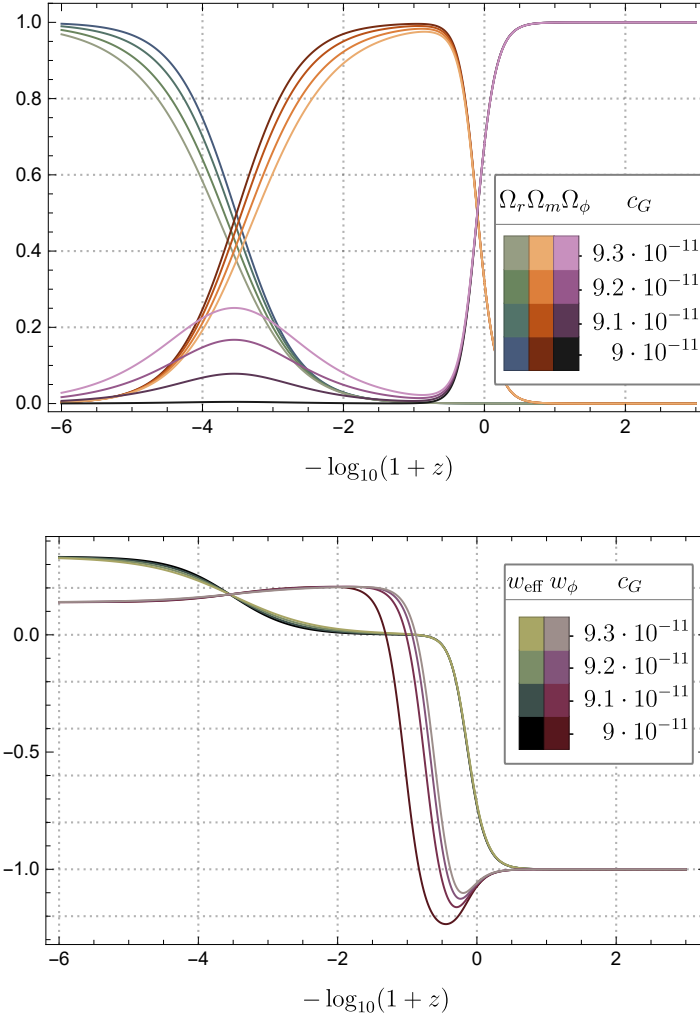


Figure 5.3: Numerical evolution for $\eta = 0.4$ and $\alpha = 0.6$ in expressions (5.54) and (5.56), respectively. In addition, the coupling constant c_K is equal to minus one, whereas c_G ranges from $9 \cdot 10^{-11}$ to $9.3 \cdot 10^{-11}$. Top panel represents the evolution of the partial energy densities for radiation, matter and the scalar field. Bottom panel shows the variation of w_{eff} and w_ϕ with the redshift.

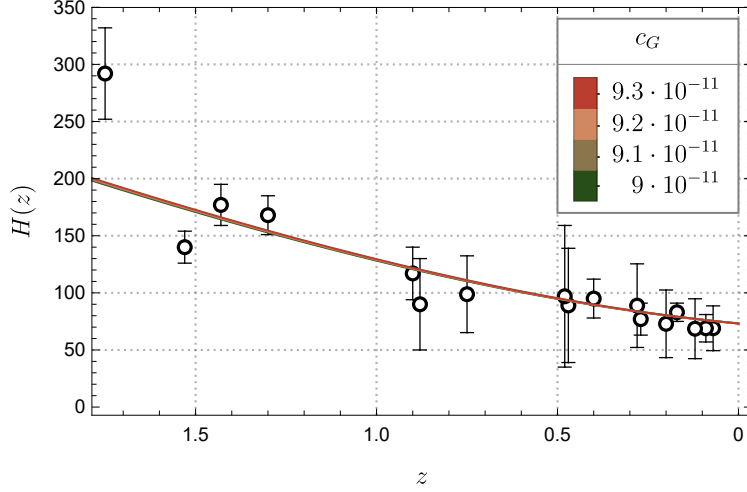


Figure 5.4: Evolution of the Hubble rate at low redshift for $\eta = 0.4$ and $\alpha = 0.6$ in expressions (5.54) and (5.56), respectively. The coupling constant c_K equals minus one, whereas c_G ranges from $9 \cdot 10^{-11}$ to $9.3 \cdot 10^{-11}$. In addition, marks on the plot correspond to direct measurements of $H(z)$ collected from references [445–449] (see also Table II in reference [450]).

a review on EDE in, for instance, reference [451]). Moreover, the resulting evolution of the Hubble rate at low redshift can, in principle, be made compatible with the current data available from direct measurements⁵; see panel 5.4. At the level of linear scalar perturbations, the ghost-free and gradient-free conditions are always satisfied (see figure 5.5), even though the model at hand shows a phantom behaviour at recent epoch as can be noted in figure 5.3. Unfortunately, as can be seen in figure 5.6, the condition (5.53) is never fulfilled for the domain of the numerical integration; that is from redshift $z_i = 10^6$ to $z_f = -0.999$. Since this bound is always violated, the signs of Z^{11} and Z^{22} will alternate between positive and negative values if $|\beta| > 1$. In that case, conditions (5.51) and (5.52) would not always be satisfied during the period of a single oscillation of the GWs. As a result, the interaction between DE fluctuations and GWs will induce (at least) a gradient instability for certain (periodic) values of the argument $\omega(t - z)$ if the amount of braiding is non-negligible. Hence, this model cannot provide a working example for the mechanism we discussed in section 5.2.2.

A second example is shown in figure 5.7. This corresponds to $\eta = 2$, $\alpha = 2$ and $c_K = -1$ in expressions (5.54) and (5.56). In this case, the coupling constant

⁵We recall that we have not fitted the parameters of the model at hand with observational data. Contrary, the previous statement comes from just comparing the resulting $H(z)$ with the current data coming from direct measurements collected from references [445–449].

c_G takes values from $4.5 \cdot 10^{-4}$ to $4.8 \cdot 10^{-4}$. The background evolution of this proxy model is still compatible with low redshift measurements, but shows some tensions with data above $z \approx 1$ for the selected values for c_G ; see upper panel in figure 5.7. The bottom panel in figure 5.7 shows the fulfilment of the condition (5.53). This condition is always satisfied in the asymptotic past of the model (within the limits of the integration domain). Unfortunately, it is consistently violated when the scalar field becomes dominant, if not even before that moment. As a result, interaction between DE fluctuations and GWs will induce (at least) a gradient instability if the amount of braiding is non-negligible.

The models represented in figures 5.3 to 5.7 illustrate the general behaviour we found for the functions (5.54) and (5.56). Even though there exist regions in the parameter-space for which $D > 0$ and $c_s^2 \geq 0$ always, the condition (5.53) is, in the best case scenario, fulfilled only for a finite time during the (past) evolution of the model. Moreover, this condition is systematically violated (at the latest) when the scalar field becomes dominant. Hence, a GWs-induced instability, like that described in reference [286] if the amount of braiding is non-negligible, seems to be inevitable for the models at hand.

However, it is important to emphasise that the numerical screening of the (η, α) -plane we have performed is not an analytic proof of the non-viability of the KGB example given by the functions (5.54) and (5.56). Moreover, a different choice for the K function may also affect the results. Nevertheless, given the naturalness of power-law functions in physics and the lack of a positive conclusion in our numerical analysis, we suspect that finding a KGB model that could implement the mechanism we discussed in section 5.2.2 for avoiding a GWs-induced instability [286] would be a rather difficult task, if not impossible.

5.3 Conclusions of the chapter

In the first part of the chapter, we have addressed the inter-connection in the shift-symmetric KGB theory between instabilities in linear cosmological perturbations and energy conditions. In the shift-symmetric k -essence scenario, we have shown how the violation of the NEC in the ϕ -fluid is responsible for the appearance of instabilities in linear scalar perturbations. When only the braiding function G is non-trivial in the KGB action (4.2), this relation turns different. Instabilities are now triggered by the sign of the EOS associated with the scalar field fluid, which precludes any viable description for DE with this scalar field theory. In the complete shift-symmetric KGB theory, this relation becomes again different. Now, stable models are possible not only for $w_\phi < 0$ but for $w_\phi + 1 < 0$ as well; see, for instance, figures 5.3 and 5.5. Hence, stable violation of the NEC by ϕ -

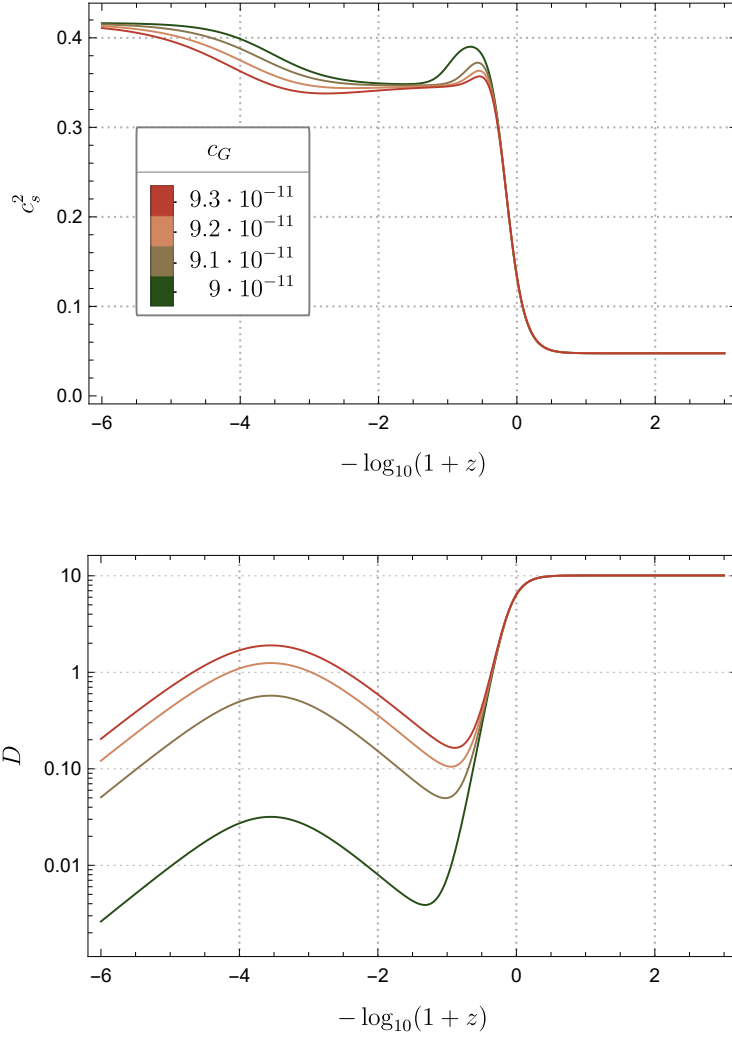


Figure 5.5: Numerical evolution for $\eta = 0.4$ and $\alpha = 0.6$ in expressions (5.54) and (5.56), respectively. In addition, the coupling constant c_K is equal to minus one, whereas c_G ranges from $9 \cdot 10^{-11}$ to $9.3 \cdot 10^{-11}$. Upper panel represents the speed of sound squared, c_s^2 , as defined in equation (5.3). Bottom figure shows the evolution of the ghost parameter D defined in equation (5.2). As can be seen, linear order perturbations (where scalar perturbations are decoupled from GWs) are always stable even though the scalar field displays a phantom behaviour at present epoch.

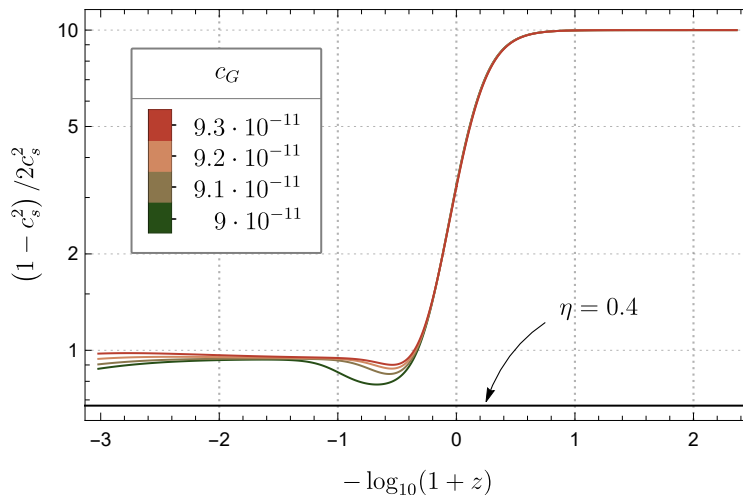


Figure 5.6: Numerical evolution for $\eta = 0.4$ and $\alpha = 0.6$ in expressions (5.54) and (5.56). Taking $c_K = -1$, the curves represent the ratio $(1 - c_s^2)/2c_s^2$ from equation (5.53) for different values of the coupling constant c_G . The horizontal line depicts the upper-bound for this ratio found in expression (5.53). Clearly the model never satisfies this bound for the domain of the numerical integration and, therefore, the interaction with GWs always introduce (at least) a gradient instability in the scalar sector.

fluid is possible. It is interesting to note, however, that for the stable phantom models we have numerically explored (and also for the phantom model reported in reference [40]) the NEC is never violated at the level of the geometry. That is, $w_{\text{eff}} + 1 \geq 0$ always. Nevertheless, it remains an open question whether this is merely a coincidence in the proposed models or a fundamental principle essential to the stability of the theory. We leave the analysis of this issue for future research.

Different considerations emerge when considering beyond linear scalar perturbations. The braiding term $G \square \phi$ in the scalar field action (2.21) has been shown to interact with GWs in such a way that it produces a ghost and/or a gradient instability in the scalar perturbations if the amount of braiding present at cosmological scales is non-negligible [286]. Motivated by the fact that the stability analysis in reference [286] was mainly performed for the special case of cubic Galileon, i.e. $G \propto X$, in the second part of this chapter we have proposed a theoretical mechanism to avoid these GW-induced instabilities for KGB models beyond cubic Galileon. This mechanism relies on having a large and positive η (quantity that measures deviations w.r.t. a linear function G) for expanding the stability region to $|\beta| \gg 1$ at low values of the speed of sound, as shown in figure 5.2. It should be mentioned, however, that the parameter β is not only proportional to the amount of braiding in the theory (through \bar{m}_1^3 or, equivalently, α_B) but to the strain ampli-

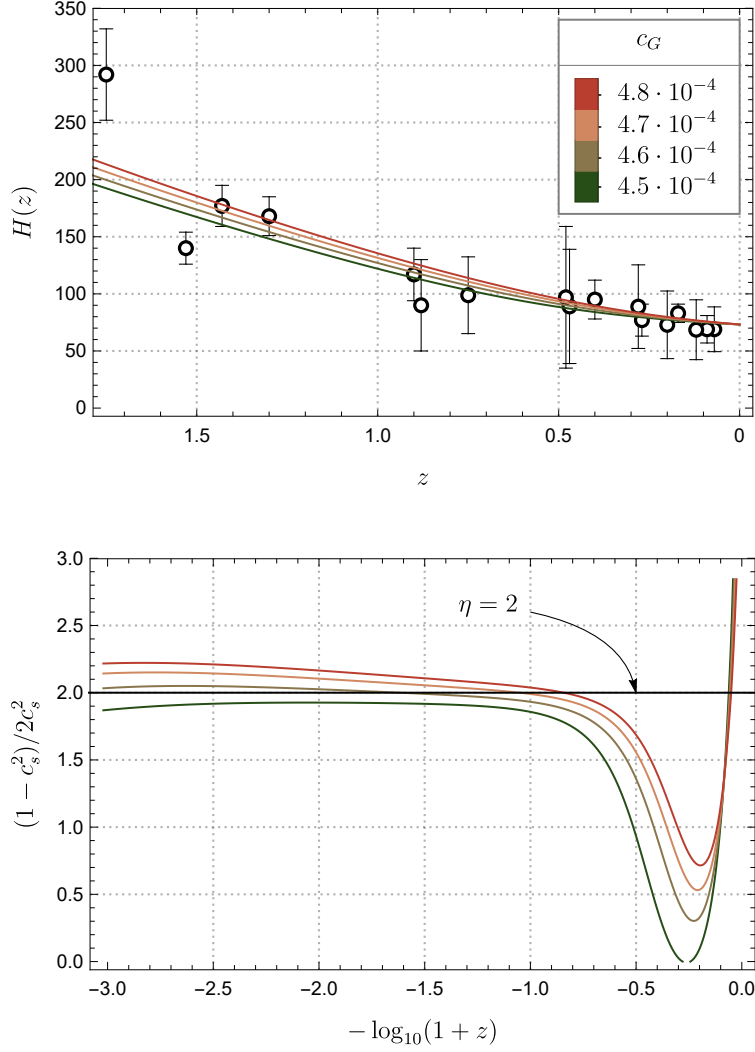


Figure 5.7: Numerical evolution for $\eta = 2$ and $\alpha = 2$ in expressions (5.54) and (5.56), respectively. In addition, the coupling constant c_K is equal to minus one, whereas c_G ranges from $4.5 \cdot 10^{-11}$ to $4.8 \cdot 10^{-11}$. Top panel shows the evolution of the Hubble rate at low redshift compared to direct measurements collected from references [445–449] (see also Table II in reference [450]). Bottom panel represents the ratio $(1 - c_s^2)/2c_s^2$ from equation (5.53). The horizontal line there depicts the upper-bound this ratio should satisfy to avoid a GWs-induced gradient instability; see inequality (5.53).

tude of the GWs as well, see equation (5.36). If observational data of GWs events with higher and higher strain amplitudes are considered, then the resulting \bar{m}_1^3 (or α_B) will still be constrained to be negligible, even though our mechanism could extend the stability region to larger values of β . In that scenario, the conclusion in reference [286] about the non-viability of the braiding at cosmological scales will be only marginally affected by the discussion we have proposed here. Nevertheless, before finally concluding that the KGB theory should not have any sizeable effects, the fate of these instabilities, once originated, should be addressed.

We have also explored whether some reasonable KGB candidate could implement the theoretical mechanism proposed here for evading GWs-induced instabilities. Unfortunately, using numerical simulations with a power-law prescription for the functions K and G we have not been able to find a working example for this effect. As we commented in section 5.2.3, the power-law choice for G provides a physically relevant case for our mechanism to work. Therefore, we consider the lack of a working example with power-law functions as a solid hint towards the non-viability of a cosmological braiding like the one present in the shift-symmetric KGB theories.

Conversely, the k -essence part in the KGB action (2.21) trivially evades the constraints coming from references [183, 286, 440]. Moreover, this scalar field theory can feature ghost-free and gradient-free scalar perturbations if the NEC is satisfied for the DE sector. As we have discussed, however, the ghost-free and gradient-free conditions for k -essence are anti-correlated when the NEC is violated. Therefore, if we were to describe a DE component that violates the NEC (a possibility that is observationally viable [128]) with a single scalar field within the k -essence theory, then we will inevitably face a ghost or a gradient instability. Whether the instability will be ghost- or gradient-like depends, ultimately, on the function K . It is also important to note that k -essence cannot produce a phantom crossing [191, 192]. Hence, the scalar field will always be phantom or non-phantom, with the stability issues this may entail in the former case. This points towards the impossibility of solving simultaneously the H_0 and S_8 tensions with late-time modifications to Λ CDM *à la* k -essence should the S_8 tension still be present in future surveys, as this resolution would demand a phantom crossing [131, 132]. See also previous works on the H_0 tension in the k -essence theory in, for instance, references [175, 193]. With this potential limitation in mind, an interesting extension of the k -essence scenario is that when more than one scalar field is present [452, 453]. In that case, the effective DE fluid can cross the phantom divide [454] even though each scalar field, namely ϕ_i , is restricted to the phantom or non-phantom regime in the same way as described in section 5.1.1.

It should be noted that the discussion presented in this chapter will be only partially affected if we allow the shift-symmetry to be (weakly) broken at some

regimes. This would introduce an explicit dependence on the scalar field ϕ in the functions K and G . The destabilising interaction between GWs and the braiding term will still occur even for $G = G(\phi, X)$ [286]. However, it would be interesting to explore whether the mechanism proposed in section 5.2.2 will have a better performance in that case. If not, then, the braiding term should not have any sizeable effect and the surviving theory will be effectively that of k -essence. For this non-shift-symmetric k -essence theory, no additional terms will appear in the formulas for the scalar field energy density and pressure, or in the equations for c_s^2 and D ; see the corresponding expressions in, for instance, reference [40]. Thus, our discussion about the linear stability of the theory shall remain the same as for the shift-symmetric case. In addition to the previous considerations, the k -essence scalar field cannot produce a phantom crossing even if $K = K(\phi, X)$; see reference [191, 192]. Therefore, the conclusions presented in section 5.1.1 shall remain unchanged.

Along this line of thought, another possible extension of the k -essence theory is that when a non-minimal coupling to gravity is allowed for the scalar field. Assuming that the external matter field are minimally coupled to the metric $g_{\mu\nu}$, the gravitational part of the total action would read

$$S_g = \int d^4x \sqrt{-g} [f(\phi)R + K(\phi, X)], \quad (5.57)$$

where the non-minimal coupling function f can only depend on the scalar field, but not on its kinetic term X . This is due to the strong restrictions on the speed of propagation of GWs; see reference [154]. Please note that this scalar field theory would also trivially evade the constraints from [286]. Nevertheless, the non-minimal coupling may introduce a fifth-force at local scales. Therefore, some mechanism should be invoked to screen this force on astrophysical scales; see, for instance, references [434, 455, 456] and references therein. This limitation may also be present in extensions of k -essence to modified theories of gravity like those discussed in, e.g., references [457–462].

Furthermore, within the spirit of analysing fundamental symmetries in order to address DE, we should also briefly mention the possibility of considering a scalar field with an action that is invariant just under transverse diffeomorphisms [450, 463–465]. In this case, one can describe phenomenology of interest for the dark sector even with a shift-symmetric field with a canonical kinetic term [450, 465]. On the other hand, one can consider more general theories invariant only under transverse diffeomorphisms [466, 467], being the most prominent example that of Unimodular Gravity [468] (see also [469–474]). Finally, as it is well-known, more general alternative theories of gravity go beyond the consideration of a scalar field to describe the dark sector [117].

Last but not least, we shall recall again that we have discussed the viability of the shift-symmetric KGB theory solely from the point of view of the stability of scalar perturbations. In doing so, we have focused on theoretical considerations only. Should any of the models studied have fulfilled our stability criteria, then the analysis of background expansion by means of the evolution of the partial energy densities and the Hubble rate (like shown in figures 5.3 and 5.7) would not be sufficient to claim the viability of the DE-candidate. In such case, a thorough analysis on the observational impact using more advanced techniques and specialised software like CLASS should be carried out; see, for instance, references [475, 476]. We leave for future research the stability of more involved KGB models and their compatibility with observational data.

Part III

Classical and quantum cosmology from
 $f(R)$ gravity

6 Phantom dark energy from $f(R)$ gravity

THE possibility of the expansion of the universe being driven by a phantom-type DE ($w_{\text{DE}} + 1 < 0$) is not observationally excluded [78, 79, 347]. Furthermore, it is even suggested by some data [128] and could help alleviate some of the current statistical tensions in the cosmological parameters (see, for instance, references [129–132]). Besides the non-standard stability properties of the phantom energy, these models may also entail some future cosmological singularities. Although this might not always be the case for phantom models; see counterexamples in [334–336]. All bound structures in the universe and ultimately the fabric of spacetime itself might be torn apart at a final BR singularity, at which the scale factor, H and \dot{H} diverge in finite cosmic time [88, 217]. Conversely, the occurrence of a future singularity may be infinitely delayed in time for a phantom DE model with an EOS parameter converging sufficiently rapidly to the cosmological constant value ($w_{\text{DE}} = -1$). This is precisely the case of the LR abrupt event [388] (see also [135, 389, 390]), where the scale factor, the Hubble rate, and its cosmic-time derivative explode at the infinite asymptotic future. Therefore, this abrupt event can be understood as a BR singularity that has been postponed indefinitely. Another characteristic abrupt event of phantom DE models is the LSBR [360]. In this scenario, the asymptotic size of the observable universe and the expansion rate diverge, but the cosmic-time derivative of the Hubble parameter converges to a constant value [360]. It should be noted, however, that even though these abrupt events take place at the infinite distant future, bound structures are destroyed in a finite time [360, 388]. See a brief summary of the phenomenology of these rip-like doomsdays in table 3.1. See also references [137, 477] for observational constraints on some phantom DE models.

The BR singularity, and the LR and the LSBR abrupt events are, in fact, intrinsic to phantom DE models. However, it is commonly believed that a consistent quantum description of the universe may prevent the appearance of classical singularities, see references [297, 298] (see also [48, 133, 134, 299, 392, 393]). The quantum fate of classical singularities can be addressed in the setup of quantum cosmology: the application of the quantum theory to the universe as a whole. Previous works in this framework have shown that the aforementioned phantom rip-like cosmological doomsdays, among other singularities such as the BB, can be avoided as a result of quantum effects emerging as the universe approaches the classical singularity [297, 302, 304] (assuming that the classical theory of gravity

is GR). However, since the same classical background evolution can be equivalently described in the context of GR or by alternative theories of gravity, it is natural to wonder whether these singularities are still avoided in the quantum realm for a different underlying classical theory of gravity. In this chapter, we discuss the classical and quantum occurrence of these three rip-like events when the description of gravity is that provided by metric $f(R)$ theories of gravity. For that purpose, we shall focus on the quantum cosmology scheme given by the WDW equation [400] being adapted for the case of $f(R)$ gravity [478], namely the modified Wheeler-DeWitt (mWDW) equation. Consequently, we explore here the possibility of avoiding the BR singularity, and the LR and the LSBR abrupt events in the realm of $f(R)$ quantum cosmology.

This chapter is based on the peer-reviewed publications [4–6]. The content is organised as follows: in section 6.1, we review some phantom DE models in GR that predict the classical appearance of future singularities and/or abrupt events. In section 6.2, we consider that the classical background cosmic evolution found in the previous section can be equivalently described in the framework of metric $f(R)$ theories of gravity, where in the latter case the accelerated expansion of the universe will have a purely geometrical origin. To that end, we briefly discuss a reconstruction method for metric $f(R)$ theories of gravity. Thereafter, in sections 6.2.1, 6.2.2 and 6.2.3, we apply this background reconstruction technique to the specific phantom DE models reviewed in section 6.1.1. Hence, we present the group of metric $f(R)$ theories of gravity predicting a classical fate *à la* BR, LR or LSBR. Section 6.3 is entirely devoted to the fate of classical singularities in $f(R)$ quantum cosmology. Therefore, we summarise the $f(R)$ quantum geometrodynamics approach in section 6.3.1. Then, the resolution of the mWDW equation corresponding to the BR, LR and LSBR doomsdays is addressed in sections 6.3.2, 6.3.3 and 6.3.4, respectively. We also discuss there the avoidance of these cosmological catastrophes by means of the DW criterion. Finally, the validity of the approximations performed to solve the mWDW equations are discussed in appendices F and G.

6.1 A phantom dark energy universe

Dark energy is the dominant cosmic component today. (Moreover, because we aim to study the far future expansion of the universe, we assume that the DE density increases, remains constant or decreases more slowly than the energy densities of other matter species.) Thus, from a practical perspective, we can neglect the contribution of the other cosmic ingredients when studying the asymptotic future

evolution. That is, we consider

$$3H^2 = \varrho, \tag{6.1}$$

$$\dot{H} = -\frac{1}{2}(p + \varrho), \tag{6.2}$$

where ϱ and p denote the energy density and pressure of the DE fluid, respectively. Let us emphasise again that this is an approximation we take for valid only above some future moment at which other constituents are sufficiently redshifted away with the cosmic expansion.

To evaluate the future fate of this DE universe, an EOS for the dark fluid must be provided. We consider the following EOS for the DE content [133, 135]

$$p = -\varrho - \mathcal{A}\varrho^\alpha, \tag{6.3}$$

which is reminiscent of a Taylor expansion around a cosmological constant and where \mathcal{A} is a positive constant¹. This EOS was first introduced in reference [133] and thoroughly discussed in terms of singularity occurrence in reference [135] (see also [134]). Here we expand the analysis performed by addressing the evolution of the scale factor a , the Hubble rate H and its cosmic time derivative \dot{H} . That is a metric classification such as the one presented in reference [48]. We advocate for this metric classification, instead of only addressing the evolution of the scale factor a and the DE density ϱ as originally done in reference [135], since different cosmic events such as the LR and LSBR cannot be differentiated in the latter picture.

From the conservation equation of a perfect fluid (e.g. equation (3.4)) and the EOS (6.3), it follows that the DE density evolves as

$$\varrho = \varrho_0 \left[1 + \frac{3(1-\alpha)\mathcal{A}}{\varrho_0^{1-\alpha}} \ln\left(\frac{a}{a_0}\right) \right]^{\frac{1}{1-\alpha}}, \tag{6.4}$$

for $\alpha \neq 1$, and

$$\varrho = \varrho_0 \left(\frac{a}{a_0}\right)^{3\mathcal{A}}, \tag{6.5}$$

for the case of $\alpha = 1$, where the subscript “0” denotes the current value of the corresponding quantity. In either case, the EOS parameter w reads

$$w = -1 - \frac{\mathcal{A}}{\varrho_0^{1-\alpha} + 3(1-\alpha)\mathcal{A} \ln\left(\frac{a}{a_0}\right)}. \tag{6.6}$$

¹Since the BR, the LR and the LSBR doomsdays are intrinsic to phantom-like DE models, we limit our discussions to a positive parameter \mathcal{A} , which leads to $w + 1 < 0$. For an analysis of the most general case, we refer the reader to the reference [135].

Note that for a non-negative parameter \mathcal{A} , the denominator in the right-hand side of equation (6.6) is always positive², whatever the value of α . Consequently, the DE content modelled by the EOS (6.3) exhibits phantom-like behaviour when the parameter \mathcal{A} is positive, as to be expected in view of the EOS (6.3).

Also note that $\alpha = 1$ and $\alpha = 1/2$ are special values on the α -line that delimit qualitatively alike cosmological behaviours [135]. This can be deduced from the time dependence of the scale factor as obtained from equations (6.1) and (6.4). That is [135]

$$\ln\left(\frac{a}{a_0}\right) = \frac{2\sqrt{\varrho_0}}{3\mathcal{A}} \left\{ \left[1 + \frac{3\mathcal{A}}{2\sqrt{\varrho_0}} \ln\left(\frac{a_\star}{a_0}\right) \right] \exp\left(\frac{\sqrt{3}\mathcal{A}}{2}(t-t_\star)\right) - 1 \right\}, \quad (6.7)$$

for the case of $\alpha = 1/2$, and [135]

$$\ln\left(\frac{a}{a_0}\right) = \frac{1}{3(\alpha-1)\varrho_0^{\alpha-1}\mathcal{A}} \left\{ 1 - \left[B - \frac{\sqrt{3}}{2}(2\alpha-1)\varrho_0^{\alpha-\frac{1}{2}}\mathcal{A}(t-t_\star) \right]^{\frac{2(\alpha-1)}{2\alpha-1}} \right\}, \quad (6.8)$$

when $\alpha = 1$. Whereas, for the general case of $\alpha \neq 1/2$ and $\alpha \neq 1$, the solution reads

$$\frac{a}{a_0} = \left[\left(\frac{a_\star}{a_0}\right)^{-\frac{3\mathcal{A}}{2}} - \frac{\sqrt{3}\varrho_0}{2}\mathcal{A}(t-t_\star) \right]^{-\frac{2}{3\mathcal{A}}}, \quad (6.9)$$

where B is a constant defined as

$$B := \left[1 + 3(1-\alpha)\varrho_0^{\alpha-1}\mathcal{A} \ln\left(\frac{a_\star}{a_0}\right) \right]^{\frac{2\alpha-1}{2(\alpha-1)}}. \quad (6.10)$$

In addition, we have denoted by t_\star some arbitrary (future) moment in the expansion history of the universe from which we can safely neglect the contribution of matter fields and, therefore, assume that DE is the only content of the cosmos. Likewise, a_\star represents the value of the scale factor at that moment.

From expression (6.7) it follows that the scale factor asymptotically approaches a double exponential growth on the cosmic time when $\alpha = 1/2$. Conversely, it evolves as some function of $t_s - t$ for $\alpha > 1/2$, being t_s the time of occurrence of the corresponding singularity. Moreover, the expression for t_s depends on the value of α . Therefore, we now proceed to discuss the different possibilities separately

²This is trivial to check when $\alpha \leq 1$. For the case of $\alpha > 1$, on the other hand, the expansion of the universe stops at a finite value of the scale factor, namely a_{\max} , such that the denominator in equation (6.6) never becomes negative; see equation (6.11).

in a similar way as in reference [135]. Those are: $\alpha > 1$, $\alpha = 1$, $1/2 < \alpha < 1$, $\alpha = 1/2$ and $\alpha < 1/2$. Additionally to the conclusion presented in reference [135], we also compute the corresponding H and \dot{H} functions in each case. This allows us to provide a complementary classification of the cosmic events found in [135] similar to that introduced in reference [48], see Table 6.1.

For the case of $\alpha > 1$, the universe reaches a maximum size given by

$$a_{\max} := a_0 \exp\left(\frac{1}{3(\alpha - 1)\varrho_0^{\alpha-1}\mathcal{A}}\right). \quad (6.11)$$

Furthermore, this size is reached in a finite time into the future

$$t_s := t_\star + \frac{2B}{\sqrt{3}(2\alpha - 1)\varrho_0^{\alpha-\frac{1}{2}}\mathcal{A}}. \quad (6.12)$$

Moment at which the Hubble rate and its comics time derivative diverge, since

$$H = \sqrt{\frac{\varrho_0}{3}} \left[\frac{\sqrt{3}}{2}(2\alpha - 1)\varrho_0^{\alpha-\frac{1}{2}}\mathcal{A}(t_s - t) \right]^{-\frac{1}{2\alpha-1}}, \quad (6.13)$$

$$\dot{H} = \frac{\varrho_0^\alpha \mathcal{A}}{2} \left[\frac{\sqrt{3}}{2}(2\alpha - 1)\varrho_0^{\alpha-\frac{1}{2}}\mathcal{A}(t_s - t) \right]^{-\frac{2\alpha}{2\alpha-1}}. \quad (6.14)$$

This asymptotic behaviour corresponds to the occurrence of a BF singularity [218, 219] (see also reference [364]). That is a type III singularity in the notation of reference [134].

Please note that the simple case of $\alpha = 1$ actually corresponds to a constant EOS parameter $w = -1 - \mathcal{A}$. Accordingly, the size of the observable universe becomes infinite at a finite time from present epoch, namely t_{rip} . This is

$$t_{\text{rip}} := t_\star + \frac{2}{\sqrt{3}\varrho_0\mathcal{A}} \left(\frac{a_\star}{a_0}\right)^{-\frac{3\mathcal{A}}{2}}, \quad (6.15)$$

see equation (6.9). Furthermore, in view of the expressions

$$H = \frac{2}{3\mathcal{A}(t_{\text{rip}} - t)}, \quad (6.16)$$

$$\dot{H} = \frac{2}{3\mathcal{A}(t_{\text{rip}} - t)^2}, \quad (6.17)$$

the Hubble rate and its cosmic time derivative also diverge at $t = t_{\text{rip}}$. Therefore, for this value of α , the universe evolves towards a classical BR singularity similar

to the one first introduced in [59, 88]. This corresponds to a type I singularity according to the notation in reference [134].

For $1/2 < \alpha < 1$, the scale factor diverge at finite cosmic time, see equation (6.8) where the ratio $2(\alpha - 1)/(2\alpha - 1)$ is now negative. This makes the $\ln a$ proportional to some power of $1/(t_{\text{rip}} - t)$. The time at which the observable universe becomes infinite is given by

$$t_{\text{rip}} := t_{\star} + \frac{2B}{\sqrt{3}(2\alpha - 1)\varrho_0^{\alpha - \frac{1}{2}}\mathcal{A}}. \quad (6.18)$$

The Hubble rate and its time derivative follows the same relations given in equations (6.13) and (6.14), respectively. Hence, these quantities also diverge along with the scale factor. Therefore, in a finite time into the future, the scale factor, the Hubble rate and \dot{H} explode. This implies that the DE density and pressure blow up, as was found in [135], even though the EOS parameter w converges to -1 from below. This event is qualitatively equivalent to a BR singularity (see the singularities classified as type I in, for example, references [48, 134, 367]). Please note that this behaviour was also found in reference [364], where it was dubbed *grand rip* (see type -1 singularities in reference [374]).

Another possible value for α corresponds to the interesting case of $\alpha = 1/2$. In this scenario, the scale factor asymptotically evolves as a double exponential function on the cosmic time, i.e., $a \approx e^{e^t}$; see equation (6.7). Accordingly, the Hubble rate and its cosmic time derivative read

$$H(t) = \sqrt{\frac{\varrho_0}{3}} \left(1 + \frac{3\mathcal{A}}{2\sqrt{\varrho_0}} \ln \frac{a_{\star}}{a_0} \right) \exp \left[\frac{\sqrt{3}}{2} \mathcal{A} (t - t_{\star}) \right], \quad (6.19)$$

$$\dot{H}(t) = \frac{A}{2} \sqrt{\varrho_0} \left(1 + \frac{3\mathcal{A}}{2\sqrt{\varrho_0}} \ln \frac{a_{\star}}{a_0} \right) \exp \left[\frac{\sqrt{3}}{2} \mathcal{A} (t - t_{\star}) \right]. \quad (6.20)$$

As a result, the scale factor, H , and \dot{H} diverge at the infinite asymptotic future. This drives the universe towards a future LR abrupt event, see classification in [48, 367]. (See also reference [389].) In fact, the EOS (6.3) with $\alpha = 1/2$ corresponds to the DE model for which the name *little rip* was first given [388], even though this cosmological behaviour was already known from before [135] (see also [389] where a fate *à la* LR was found in brane cosmology and before that in some modified theories of gravity [391]).

Finally, for the case of $\alpha < 1/2$, the scale factor obeys the relation given in equation (6.8). However, since now the ratio $2(\alpha - 1)/(2\alpha - 1)$ is positive, then the equation for $\ln a$ reduces to a certain polynomial on the cosmic time. This makes the expansion of the observable universe last for ever. Hence, no finite

α	t_s	a_s	H_s	\dot{H}_s	Event
$1 < \alpha$	Finite	Finite	∞	∞	Big freeze
$\frac{1}{2} < \alpha \leq 1$	Finite	∞	∞	∞	Big rip
$0 < \alpha \leq \frac{1}{2}$	∞	∞	∞	∞	Little rip
$\alpha \leq 0$	∞	∞	∞	Finite	LSBR

Table 6.1: Classification of the singularities and abrupt events for the phantom DE model given by the general EOS (6.3) with \mathcal{A} positive; cf. reference [135]. The classification is performed according to the value of the parameter α , the time of occurrence of the singular behaviour t_s , and the value of the scale factor, the Hubble rate and \dot{H}_s at the event. Please note that since the BR and grand rip [364] singularities have qualitatively the same behaviour in terms of those quantities, we do not address the possible differences between both events in the following classification. Hence, we keep the term *big rip* for both of them.

time singularities are present in this case. The Hubble rate and its cosmic time derivative read

$$H = \sqrt{\frac{\varrho_0}{3}} \left[B + \frac{\sqrt{3}(1-2\alpha)\mathcal{A}}{2\varrho_0^{\frac{1}{2}-\alpha}}(t-t_*) \right]^{\frac{1}{1-2\alpha}}, \quad (6.21)$$

$$\dot{H} = \frac{\mathcal{A}}{2} \varrho_0^\alpha \left[B + \frac{\sqrt{3}(1-2\alpha)\mathcal{A}}{2\varrho_0^{\frac{1}{2}-\alpha}}(t-t_*) \right]^{\frac{2\alpha}{1-2\alpha}}. \quad (6.22)$$

For $0 < \alpha < 1/2$, both quantities tend to infinity at the infinite asymptotic future, thus, leading to the occurrence of a LR abrupt event. On the contrary, \dot{H} remains constant for $\alpha = 0$, or shrinks to zero when $\alpha < 0$. This behaviour corresponds to a final fate *à la* LSBR, see reference [360]. Please note that since the DE density (6.4) grows unbounded in both abrupt events, the LR and the LSBR, the distinction between these events could not be noticed analysing only the asymptotic evolution of a and ϱ as originally done in reference [135]. Also interesting to note that given some entire number n , all the higher order derivatives of H up to the n -th order diverge when $\alpha = (n-1)/2n$.

We conclude, therefore, that the phantom DE models described by the EOS (6.3) with a positive parameter \mathcal{A} entail a great variety of cosmological singularities and abrupt events. We summarise the results from reference [135] and our new findings in table 6.1.

6.1.1 Cosmological constraints

Since we are mainly interested in the classical and quantum fate of the BR, the LR and the LSBR events in metric $f(R)$ theories of gravity, we should now restrict our attention to some particular phantom DE models on which to apply the reconstruction techniques in the next sections. Therefore, hereafter we shall consider only the following phantom DE models when addressing the occurrence of these cosmic events:

- For the BR singularity we consider the phantom DE model with a constant EOS parameter $w < -1$ [217]. This model corresponds to the choice of $\alpha = 1$ in the more general EOS (6.3) studied in the previous section.
- For a DE model with a future LR abrupt event, we select the EOS for DE described in reference [388], which corresponds to the case $\alpha = 1/2$ in (6.3).
- For a universe doomed to evolve towards a LSBR abrupt event, we consider the DE content to be described by the EOS (6.3) with $\alpha = 0$. This LSBR was first introduced in reference [360].

Note that the BR model here considered is just a subcase of the more general w CDM scenario, which has been thoroughly analysed in the literature (see, for example, references [78, 79, 120–126], among others). More importantly, these specific phantom DE models have been shown to be compatible with the current observational data; see, for instance, references [78, 79, 120, 137, 388, 477, 479].

In the following, for the sake of concreteness, we shall consider the cosmological constraints obtained in reference [137] when binding those DE models with observational data. Thus, the results presented in the incoming sections are subjected to the observational constraints on the parameter \mathcal{A} presented in reference [137]. These constraints are summarised in table 6.2. Please note that the small values for \mathcal{A} there obtained suggest that tiny deviations from the Λ CDM scenario are, in fact, the observationally preferred situation today [137]. Nevertheless, we recall that the asymptotic evolution of these DE models is not that of a dS universe, since the corresponding H and \dot{H} do not converge to a constant value but might diverge. In the next section, we will obtain the group of metric $f(R)$ theories of gravity able to reproduce the same asymptotic expansion history, which in GR corresponds to these particular phantom DE models.

6.2 Phantom dark energy models in $f(R)$ cosmology

For a given cosmological background evolution in GR it is possible to find a family of alternative theories of gravity that lead to the same expansion history. The

	α	\mathcal{A}
BR	1	0.0276 ± 0.0240
LR	$\frac{1}{2}$	$(2.75 \pm 1.30) \times 10^{-28}$
LSBR	0	$(2.83 \pm 4.17) \times 10^{-54}$

Table 6.2: Best fit found in reference [137] for the phantom DE models discussed in section 6.1.1, where \mathcal{A} is dimensionless for the case of the BR (see also [78, 79]), and has units of inverse of meter and inverse of square meter for the LR and LSBR models, respectively.

group of techniques used to perform such background reconstruction task are dubbed as *reconstruction methods* (for a review of the topic see, for instance, reference [480] and references therein). In this part of the chapter, we shall focus our attention on reconstruction methods within the scheme of metric $f(R)$ theories of gravity. Hence, we look for a metric $f(R)$ theory of gravity able to reproduce the same asymptotic super-accelerated expansion profile to that of the relativistic model filled with phantom DE with the EOS given in equation (6.3), for the values of α selected in section 6.1.1. It is worth noting that whereas in GR the accelerated phase is attributed to the existence of an exotic form of energy with a negative pressure (DE), in the setup of $f(R)$ theories of gravity the same expansion has a rather geometrical origin. Furthermore, as the relativistic model with the EOS (6.3) expands the cosmos towards some future doomsdays, then the resulting metric $f(R)$ theory of gravity will lead to the same classical fate for the spacetime. Previous works on reconstruction techniques in $f(R)$ gravity can be found in, for instance, references [480–486]. See also references [5, 6, 111, 422, 487] for successful reconstruction of phantom DE-driven rip-like events in metric $f(R)$ theories of gravity.

Hereon, we shall refer to two cosmological evolutions as equivalent at the background level if the corresponding Hubble functions H (and, therefore, \dot{H} , R and \dot{R}) are identical [111]. In GR, the (asymptotic) expansion of a flat FLRW universe is ruled by the Friedmann (6.1) and Raychaudhuri (6.2) equations. Accordingly, the scalar curvature reads

$$R = 6 \left(\dot{H} + 2H^2 \right) = \varrho - 3p, \quad (6.23)$$

where ϱ and p denotes the total energy density and pressure, respectively. Additionally, from the continuity equation for the perfect fluid and the Friedmann equation, it follows that

$$\dot{\varrho} = -\sqrt{3}\varrho(p + \varrho), \quad (6.24)$$

$$\dot{p} = -\sqrt{3}\varrho(p + \varrho) \frac{dp}{d\varrho}, \quad (6.25)$$

where we have assumed a barotropic pressure $p = p(\varrho)$. Consequently, the cosmic time derivative of the scalar curvature R reads

$$\dot{R} = -\sqrt{3\varrho}(p + \varrho) \left(1 - 3\frac{dp}{d\varrho}\right). \quad (6.26)$$

On the other hand, for the gravitational interaction being that provided by metric $f(R)$ theories of gravity, the evolution of the universe is described by the action

$$S = \frac{1}{2} \int d^4x \sqrt{-g} f(R) + S_{\text{ext}}, \quad (6.27)$$

where S_{ext} stands for the minimally coupled matter fields. In this framework, the field equations no longer coincide with the Friedmann and Raychaudhuri equations of GR. In fact, the modified Friedmann equation reads

$$3H^2 \frac{df}{dR} = \frac{1}{2} \left(R \frac{df}{dR} - f \right) - 3H\dot{R} \frac{d^2f}{dR^2} + \varrho_{\text{ext}}, \quad (6.28)$$

being ϱ_{ext} the energy density of the minimally coupled matter fields. Since we are interested in a metric $f(R)$ theory able to reproduce the same background cosmological expansion as a certain relativistic model, then the preceding expression can be considered as a differential equation for some, *a priori* unknown, function $f(R)$, where the coefficients are already fixed. That is, when the geometrical quantities involved in equation (6.28) are set to be equal to those of the GR model that we want to reproduce. Moreover, as we are mainly interested on the asymptotic behaviour of the universe, we can also neglect the matter part which will be quickly redshifted in the future, that is, ϱ_{ext} . In doing so, the asymptotic future background cosmological expansion of the resulting metric $f(R)$ theory of gravity will be equivalent to that provided by the phantom dominated relativistic model.

In the following sections we present the most general solution to this reconstruction procedure when considering the EOS given in expression (6.3) for the different values of α discussed in section 6.1.1. It is worth to point out that the resulting $f(R)$ theories must be understood as useful asymptotic models for the study of the behaviour of the universe near classical singularities, since a more realistic background reconstruction would imply the non-cancellation of the matter and/or spatial curvature contributions to the respective field equations.

6.2.1 The BR singularity in $f(R)$ gravity

For the BR singularity we considered the case of $\alpha = 1$ in the DE general EoS (6.3). This is

$$p = -(1 + \mathcal{A})\varrho. \quad (6.29)$$

For that specific value of α , the cosmic time derivative of the Hubble rate can be re-expressed as

$$\dot{H} = \frac{3}{2}\mathcal{A}H^2, \quad (6.30)$$

compare equations (6.16) and (6.17). Consequently, the scalar curvature and its cosmic time derivative reduce to

$$R = 3(4 + 3\mathcal{A})H^2, \quad (6.31)$$

$$\dot{R} = 9(4 + 3\mathcal{A})\mathcal{A}H^3, \quad (6.32)$$

respectively. Substituting these quantities into the modified Friedmann equation (6.28) results in

$$R^2 f_{RR} - \frac{2 + 3\mathcal{A}}{6\mathcal{A}} R f_R + \frac{4 + 3\mathcal{A}}{6\mathcal{A}} f = 0, \quad (6.33)$$

where we recall the use of the compact notation $f_R := df/dR$ and $f_{RR} := d^2f/dR^2$. The most general solution for the function $f(R)$ was already obtained in reference [111]. That is

$$f(R) = c_+ R^{\gamma_+} + c_- R^{\gamma_-}, \quad (6.34)$$

being c_+ and c_- arbitrary integration constants and

$$\gamma_{\pm} := \frac{1}{2} \left\{ 1 + \frac{2 + 3\mathcal{A}}{6\mathcal{A}} \pm \sqrt{\left[1 + \frac{2 + 3\mathcal{A}}{6\mathcal{A}} \right]^2 - \frac{2(4 + 3\mathcal{A})}{3\mathcal{A}}} \right\}, \quad (6.35)$$

a parameter labelling different models. In general, this parameter may take complex values. However, for $\{\mathcal{A} \leq (10 - 4\sqrt{6})/3\} \cup \{\mathcal{A} \geq (10 + 4\sqrt{6})/3\}$, both branches are real valued. Please note that this is precisely the case for the values of \mathcal{A} showed in table 6.2. Hence, taking the observational constraints [137] as a reference value for \mathcal{A} , both branches of the parameter γ_{\pm} are real valued.

6.2.2 The LR in $f(R)$ gravity

For the LR abrupt event, we consider the EOS (6.3) for DE with $\alpha = 1/2$. This run as follows

$$p = -\varrho - \mathcal{A}\sqrt{\varrho}, \quad (6.36)$$

where we recall that the parameter \mathcal{A} is observationally constrained in table 6.2. Note that for this choice of α , the Hubble rate in equation (6.19) is an exponential function on the cosmic time. Subsequently, its cosmic time derivative is

proportional to itself. Thus, for the sake of simplicity, we denoted by μ that proportionality constant. That is

$$\dot{H} = \mu H, \quad (6.37)$$

where we have defined

$$\mu := \frac{\sqrt{3}}{2} \mathcal{A}. \quad (6.38)$$

The curvature scalar and its cosmic time derivative in terms of the Hubble rate are

$$R = 6H(\mu + 2H), \quad (6.39)$$

$$\dot{R} = 6\mu H(\mu + 4H), \quad (6.40)$$

respectively. As noted in reference [487] (see also [4, 5]), the modified Friedmann equation (6.28) simplifies when rewritten in terms of H instead of the scalar curvature R . Thus, we need to solve

$$\mu H^2 (\mu + 4H) f_{HH} - [4\mu H^2 + H(\mu + H)(\mu + 4H)] f_H + (\mu + 4H)^2 f = 0, \quad (6.41)$$

where we recall that ϱ_{ext} has been neglected. The most general solution to the above differential equation is [487]

$$f(H) = \tilde{c}_1 (H^4 - 5\mu H^3 + 2\mu^2 H^2 + 2\mu^3 H) + \tilde{c}_2 \left[\mu H (\mu^2 + 4\mu H - H^2) e^{\frac{H}{\mu}} + (H^4 - 5\mu H^3 + 2\mu^2 H^2 + 2\mu^3 H) \text{Ei} \left(\frac{H}{\mu} \right) \right], \quad (6.42)$$

being \tilde{c}_1 and \tilde{c}_2 integration constants and Ei the exponential integral function (see definition, e.g., in 5.1.2 of reference [488]). In order to obtain the final $f(R)$ expression, relation (6.39) must be inverted. This inversion reads

$$H = \frac{1}{12} \left(-3\mu \pm \sqrt{9\mu^2 + 12R} \right). \quad (6.43)$$

At first glance, it seems that this transformation cannot be defined unambiguously. However, since the phantom DE density (6.4) increases with the expansion of the universe, the corresponding Hubble rate (6.19) and scalar curvature (6.39) must grow as well. Hence, only the positive branch in the preceding expression applies.

Therefore, the most general family of metric $f(R)$ theories of gravity predicting the occurrence of the LR abrupt event given by (6.36) reads [487]

$$\begin{aligned}
f(R) = & c_1 \left[27\mu^4 + 150\mu^2 R - \mu (9\mu^2 + 12R)^{\frac{3}{2}} + 2R^2 \right] \\
& + c_2 \left\{ \mu \left(-3\mu^2 - 2R + 9\mu\sqrt{9\mu^2 + 12R} \right) \right. \\
& \times \left(-3\mu + \sqrt{9\mu + 12R} \right) \exp \left(-\frac{1}{4} + \frac{1}{4}\sqrt{1 + \frac{4R}{3\mu}} \right) \\
& \left. + \left[27\mu^4 + 150\mu^2 R - \mu (9\mu^2 + 12R)^{\frac{3}{2}} + 2R^2 \right] \text{Ei} \left(-\frac{1}{4} + \frac{1}{4}\sqrt{1 + \frac{4R}{3\mu}} \right) \right\}
\end{aligned} \tag{6.44}$$

being c_1 and c_2 integration constants related to \tilde{c}_1 and \tilde{c}_2 in expression (6.42); see also references [4, 5].

6.2.3 The LSBR in $f(R)$ gravity

The selected DE model in this case corresponds to $\alpha = 0$ in the EOS (6.3), which reduces to [360]

$$p = -\rho - \mathcal{A}, \tag{6.45}$$

where \mathcal{A} takes the value shown in table 6.2. In this scenario, the cosmic time derivative of the Hubble rate remains constant since

$$\dot{H} = \frac{\mathcal{A}}{2}, \tag{6.46}$$

compare with equation (6.22). Hence, the scalar curvature and its cosmic time derivative reduce to

$$R = 12H^2 + 3\mathcal{A}, \tag{6.47}$$

$$\dot{R} = 12\mathcal{A}H. \tag{6.48}$$

Consequently, the modified Friedmann equation (6.28) becomes [6]

$$3\mathcal{A}(R - 3\mathcal{A})f_{RR} - \frac{1}{4}(R + 3\mathcal{A})f_R + \frac{1}{2}f = 0, \tag{6.49}$$

whose most general solution reads [6]

$$f(R) = c_3 (9\mathcal{A}^2 - 18\mathcal{A}R + R^2) + c_4 \left(\frac{R - 3\mathcal{A}}{12\mathcal{A}} \right)^{\frac{3}{2}} {}_1F_1 \left(-\frac{1}{2}; \frac{5}{2}; \frac{R - 3\mathcal{A}}{12\mathcal{A}} \right), \tag{6.50}$$

where c_3 and c_4 are integration constants and ${}_1F_1$ is the confluent hypergeometric function or Kummer's function; see definition in chapter 13 of reference [488]. We recall that the possible values of \mathcal{A} we shall consider here are portrayed in table 6.2.

6.2.4 Viability and local system tests

It is a well-known fact that local tests pose rather tight constraints on the metric formulation of $f(R)$ theories of gravity (see, for example, references [236–242]). Thus, any candidate for a reliable alternative to GR should pass or, somehow, evade these low-curvature-regime tests (see also [246–251] for an interesting discussion). However, the metric $f(R)$ models presented here were expressly built to reproduce a high curvature regime very different from that of (an effective) Λ CDM. Please note that the contributions of other species to equations (1.22) and (6.28) different from DE have been de facto ignored. Therefore, the resulting $f(R)$ theories obtained here must be seen as useful asymptotic models for the theoretical evaluation of the quantum fate of classical singularities rather than complete proposals for viable alternatives to GR at all scales. For example, it would be possible, in principle, to have a given $f(R)$ function that satisfies these local tests and asymptotically behaves like one of the $f(R)$ functions studied here.

6.3 $f(R)$ quantum geometrodynamics

Spacetime singularities seem to be an inevitable prediction of the classical theory of gravity. Nevertheless, it is commonly believed that a complete and consistent quantum description of the universe may prevent the appearance of classical singularities, see references [297, 298] (see also [48, 133, 134, 299, 392, 393]). Even though there is a lack of consensus on what is the correct quantum theory of gravity, the application of ordinary quantum mechanics to the universe as a whole leads to an interesting framework for addressing the issue of classical singularities. This is known as quantum cosmology. Among the different proposals to quantize cosmological backgrounds, here we will focus on the framework of quantum geometrodynamics based on the WDW equation (see section 3.3 for an introduction). In this approach, the avoidance of classical singularities in the quantum realm can be addressed through the DW criterion. That is, the classical singularity is potentially avoided if the wave function of the universe vanishes in the nearby configuration space. This criterion is based on a generalization of the interpretation of the wave function in ordinary quantum theory, where the wave function is the fundamental building block for any observable. Consequently, regions of the configuration space that lie outside of the support of Ψ are, therefore, irrelevant

in practice³. It should be noted, however, that the non-vanishing of the wave function does not necessarily entail a singularity. Therefore, the DW criterion can only be a sufficient but not necessary criterion for the avoidance of singularities. This criterion has been successfully applied in several cosmological scenarios, see, e.g., references [4, 6, 48, 297, 299, 302, 304, 416–418, 422] among others.

6.3.1 Modified Wheeler-DeWitt equation

Following the ideas presented in reference [478], the WDW equation must be adapted to the framework of $f(R)$ theories of gravity. It is worth noting that when investigating the canonical quantization of an $f(R)$ theory we are interpreting that theory as a fundamental theory of gravity, rather than an effective framework coming from a quantum gravity proposal. In this section, we shall show how the formalism of quantum geometrodynamics can be adopted to perform such quantization. The resulting scheme is known as $f(R)$ quantum geometrodynamics.

We start from the action (6.27) of metric $f(R)$ theories of gravity in the so-called Jordan frame. For a flat FLRW background metric, and neglecting the external matter fields, the action can be re-expressed as

$$S = \frac{1}{2} \int dt \mathcal{L}(a, \dot{a}, \ddot{a}), \tag{6.51}$$

where the point-like Lagrangian density reads

$$\mathcal{L}(a, \dot{a}, \ddot{a}) = \mathcal{V}_{(3)} a^3 f(R), \tag{6.52}$$

denoting by $\mathcal{V}_{(3)}$ the spatial three-dimensional volume. Please note that metric $f(R)$ theories of gravity have an additional degree of freedom when compared with GR (see Einstein's and Jordan's frame formulation in [489–492] and references therein). Consequently, a new variable can be introduced for the canonical quantization of these alternative theories of gravity. Furthermore, this new variable can be selected in such a way to remove the dependence of the action (6.51) on the second derivatives of the scale factor. Hence, following the line of reasoning presented in reference [478], we select the scalar curvature, R , to be the new variable. Then, the action (6.51) becomes

$$S = \frac{1}{2} \int dt \mathcal{L}(a, \dot{a}, R, \dot{R}). \tag{6.53}$$

³Alternatively to this interpretation, the wave function Ψ can be linked in a heuristic way with the probability distribution [413]. In that sense, having a vanishing wave function could be interpreted as having zero probability of reaching that point in the configuration space. Nevertheless, this interpretation is based on the existence of squared integral functions and a consistent probability interpretation of the wave function. The problem is that these assumptions would require a minisuperspace with a proper Hilbert space nature, and that is not obvious to be always doable for a quantum cosmology based on the WDW equation.

However, since the scalar curvature and the scale factor are not independent (at the classical level), their relation needs to be properly introduced in the theory via a Lagrange multiplier, $\bar{\mu}$, for the classical constraint $R = R(a, \dot{a}, \ddot{a})$ given in equation (1.22). Thence,

$$\mathcal{L} = \mathcal{V}_{(3)} a^3 \left\{ f(R) - \bar{\mu} \left[R - 6 \left(\frac{\ddot{a}}{a} + \frac{\dot{a}^2}{a^2} \right) \right] \right\}. \quad (6.54)$$

The Lagrange multiplier can be determined by varying the action w.r.t. the scalar curvature. This leads to

$$\bar{\mu} = f_R(R). \quad (6.55)$$

Accordingly, the point-like Lagrangian density (6.54) can be reformulated as

$$\mathcal{L}(a, \dot{a}, R, \dot{R}) = \mathcal{V}_{(3)} \left\{ a^3 \left[f(R) - R f_R(R) \right] - 6a^2 f_{RR}(R) \dot{a} \dot{R} - 6a f_R(R) \dot{a}^2 \right\}. \quad (6.56)$$

For the sake of the quantization procedure, the derivative part of the above point-like Lagrangian can be diagonalized by the introduction of a new set of variables [478]. These are

$$q := a \sqrt{R_\star} \left(\frac{f_R}{f_{R_\star}} \right)^{\frac{1}{2}}, \quad (6.57a)$$

$$x := \frac{1}{2} \ln \left(\frac{f_R}{f_{R_\star}} \right), \quad (6.57b)$$

being R_\star a constant needed for the change of variables to be well-defined. There are different proposals among the existing literature for the value of this constant, see, for instance, references [5, 6, 422, 478]. In this chapter we adopt the convention discussed in reference [5], where R_\star is defined as the value of the curvature scalar evaluated at some future scale factor $a = a_\star$ on which the description of the universe (in GR) by means of DE only becomes appropriate. That is

$$R_\star := R(a, \dot{a}, \ddot{a}) \Big|_{a=a_\star}, \quad (6.58)$$

where $R(a, \dot{a}, \ddot{a})$ obeys the classical relation (1.22). Furthermore, for the sake of concreteness, we can hereafter safely assume $a_\star = 100a_0$. Since at that moment in the expansion the matter content will be diluted by a factor of 10^{-6} w.r.t. the present concentration and, therefore, $\Omega_{DE} \approx 1$. Please note that from this definition it follows $R > R_\star$, since the scalar curvature asymptotically approaches an increasing function with the expansion of the universe. For different definitions of

R_* see references [6, 422, 478]. In these new variables, expression (6.56) transforms into

$$\mathcal{L}(q, \dot{q}, x, \dot{x}) = \mathcal{V}_{(3)} \left(\frac{R_* f_R}{f_{R_*}} \right)^{-\frac{3}{2}} q^3 \left[f - 6f_R \frac{\dot{q}^2}{q^2} - Rf_R + 6f_R \dot{x}^2 \right], \quad (6.59)$$

where f and f_R are now understood as functions of x . This form of the Lagrangian is already suitable for the quantization procedure.

Since the kinetic part of the point-like Lagrangian has been diagonalized, the derivation of the corresponding Hamiltonian is straightforward. The conjugate momenta are

$$P_q = \frac{\partial \mathcal{L}}{\partial \dot{q}} = -12\mathcal{V}_{(3)} R_*^{-\frac{3}{2}} f_{R_*}^{\frac{3}{2}} f_R^{-\frac{1}{2}} q \dot{q}, \quad (6.60)$$

$$P_x = \frac{\partial \mathcal{L}}{\partial \dot{x}} = 12\mathcal{V}_{(3)} R_*^{-\frac{3}{2}} f_{R_*}^{\frac{3}{2}} f_R^{-\frac{1}{2}} q^3 \dot{x}. \quad (6.61)$$

Then, the Hamiltonian density reads

$$\mathcal{H} = -\mathcal{V}_{(3)} q^3 \left(\frac{R_* f_R}{f_{R_*}} \right)^{-3/2} \left\{ f - Rf_R + \frac{6R_*^3}{(12)^2 \mathcal{V}_{(3)}^2 f_{R_*}^3} \frac{f_R^2}{q^4} \left[P_q^2 - \frac{P_x^2}{q^2} \right] \right\}. \quad (6.62)$$

For the quantization of the theory, we assume the usual procedure

$$P_q \rightarrow -i\hbar \frac{\partial}{\partial q}, \quad (6.63)$$

$$P_x \rightarrow -i\hbar \frac{\partial}{\partial x}. \quad (6.64)$$

Therefore, the Hamiltonian (6.62) of the classical system is promoted to a quantum operator acting on the wave function Ψ describing the quantum state of the system. Consequently, the classical Hamiltonian constraint becomes the mWDW equation for the wave function Ψ of the universe [394, 400, 478]. That is

$$\hat{\mathcal{H}}\Psi = 0. \quad (6.65)$$

After simple manipulations, the preceding expression can be cast in the form of the hyperbolic differential equation [478]

$$\left[\hbar^2 q^2 \frac{\partial^2}{\partial q^2} - \hbar^2 \frac{\partial^2}{\partial x^2} - V(q, x) \right] \Psi(q, x) = 0, \quad (6.66)$$

where the factor-ordering parameter has been set to zero [478]. The effective potential entering the preceding equation is given by⁴

$$V(q, x) = \frac{q^6}{6\lambda^2 R_* f_{R_*}} (f - Rf_R) e^{-4x}, \quad (6.67)$$

⁴See reference [4] for the case of non-vanishing spatial curvature.

being $\lambda := R_*/(12\mathcal{V}_{(3)}f_{R_*})$. Please note that for a given $f(R)$ expression, the variables q and x are univocally fixed. Then, the relation in (6.57b) must be reversed to express f and Rf_R in terms of x . However, this may not always be possible analytically, limiting the non-numerical evaluation of the mWDW equation (6.66) to only certain $f(R)$ theories. In the next sections, we will address the solutions to the mWDW equation (6.66) when considering the $f(R)$ expressions previously found sections 6.2.1, 6.2.2 and 6.2.3. We recall that these metric $f(R)$ theories of gravity lead to the same asymptotic background expansion as their respective phantom DE models in GR and, therefore, they predict (at the classical level) singular cosmological behaviours.

Before proceeding further, we want to address some comments on the structure of the mWDW equation (6.66). First, we want to emphasise the well-known ambiguity in the factor ordering in equation (6.66), i.e., we could have chosen a different factor ordering when applying the quantization procedure on the Hamiltonian of the classical theory, which could have led to a different wave function of the universe. It was argued in reference [478], however, that a variation of the factor ordering affects only the pre-exponential factor of the semi-classical wave function. Moreover, in references [302, 304, 493, 494] (see also reference [495]) the DW criterion was found to be satisfied independently of the chosen factor ordering for some particular models related to the topic discussed in this chapter. Based on these results, we consider that the actual factor ordering in the mWDW equation is not important for evaluating the DW criterion at the classical singularities, which is our primary goal. Secondly, we want to highlight that the mWDW equation (6.66) is a globally hyperbolic differential equation. That is to say, the signature of the minisuperspace DeWitt metric,

$$G^{AB} = \begin{pmatrix} q^2 & 0 \\ 0 & -1 \end{pmatrix}, \quad (6.68)$$

is $(+, -)$. This is quite different to what happens in GR when the DE content is described by a minimally coupled phantom scalar field. In that case, the DeWitt metric has a positive signature and, therefore, the WDW equation is of an elliptic type. Examples of these models can be found, for instance, in references [297, 299, 302, 304]. Additionally, a change of signature in the WDW equation has also been noticed in the presence of non-minimally coupled scalar fields [412].

6.3.2 The BR in $f(R)$ quantum cosmology

In view of expression (6.35), only the negative branch gives the expected limit to a dS universe when the parameter \mathcal{A} shrinks to zero; i.e. $f(R) \propto R^2$. On the contrary, the exponent γ_+ diverges when \mathcal{A} vanishes. Since small deviations from

the EOS of a cosmological constant are the observationally preferred situation today [137] (see also references [78, 79, 120–126], among others), hereafter we consider only the negative branch of the solution presented in equation (6.34). This is, we assume $c_+ = 0$ in expression (6.34). Therefore, in this section, we quantize a subclass of the more general family of metric $f(R)$ theories of gravity predicting the classical occurrence of a BR singularity. That is

$$f(R) = c_- R^{\gamma^-}. \quad (6.69)$$

In the following of this section, we drop the subindex “-” for the sake of the notation but keeping in mind that the preceding expression corresponds only to one of the two independent solutions obtained from the reconstruction procedure. Additionally, note that cosmological constraints on the model [137] (see also references [78, 79]) satisfy the condition $\mathcal{A} \leq (10 - 4\sqrt{6})/3 \approx 0.067$. As a result, those constraints favour a real valued exponent in equation (6.69); see discussion below equation (6.35). Hence, we shall consider that the aforementioned exponent is real for the values of \mathcal{A} of physical interest. Please note that the quantum fate of the BR singularity in $f(R)$ gravity has already been studied in the literature for some particular values for \mathcal{A} , finding that the DW criterion can be satisfied, see reference [422].

For the selected $f(R)$ theory of gravity, the change of variables in equation (6.57) reads

$$q = a\sqrt{R_\star} \left(\frac{R}{R_\star} \right)^{\frac{\gamma-1}{2}}, \quad (6.70a)$$

$$x = \frac{1}{2} \ln \left(\frac{R}{R_\star} \right)^{\gamma-1}. \quad (6.70b)$$

Moreover, from the evolution equations for the Hubble rate and its cosmic time derivative, and the definition adopted in expression (6.58), it follows that the constant R_\star is

$$R_\star = \varrho_0(4 + 3\mathcal{A})100^{3\mathcal{A}}. \quad (6.71)$$

Accordingly, the effective potential (6.67) entering the mWDW equation (6.66) becomes

$$V(q, x) = -\frac{\gamma-1}{6\lambda^2\gamma} e^{-Cx} q^6, \quad (6.72)$$

where, for the sake of compactness, we have adopted the notation of

$$C := 2\frac{\gamma-2}{\gamma-1}, \quad (6.73)$$

a constant. Thus, the mWDW equation (6.66) reads [422]

$$\left[\hbar^2 q^2 \frac{\partial^2}{\partial q^2} - \hbar^2 \frac{\partial^2}{\partial x^2} + \frac{\gamma - 1}{6\lambda^2 \gamma} e^{-Cx} q^6 \right] \Psi(q, x) = 0. \quad (6.74)$$

Written in these minisuperspace variables, the effective potential depends explicitly on both variables. This dependence can be *reduced* when considering the following change of variables [422] (see also reference [304])

$$q = r(z) \theta, \quad (6.75a)$$

$$x = z, \quad (6.75b)$$

from which it follows that [304]

$$\frac{\partial^2}{\partial q^2} = r^{-2} \frac{\partial^2}{\partial \theta^2}, \quad (6.76)$$

$$\frac{\partial^2}{\partial x^2} = \left(\frac{r'}{r} \right)^2 \left[\theta^2 \frac{\partial^2}{\partial \theta^2} + \theta \frac{\partial}{\partial \theta} \right] - 2 \frac{r'}{r} \theta \frac{\partial}{\partial \theta} \frac{\partial}{\partial z} + \left[\left(\frac{r'}{r} \right)^2 - \frac{r''}{r} \right] \theta \frac{\partial}{\partial \theta} + \frac{\partial^2}{\partial z^2}, \quad (6.77)$$

Then, the potential term will only depend on θ for the choice of $r(z) = e^{Cz/6}$ [422]. Accordingly, the mWDW equation (6.74) transforms to [422] (see also [4])

$$\left[\left(1 - \frac{C^2}{36} \right) \hbar^2 \theta^2 \frac{\partial^2}{\partial \theta^2} - \hbar^2 \frac{\partial^2}{\partial z^2} + \frac{C}{3} \hbar^2 \theta \frac{\partial}{\partial \theta} \frac{\partial}{\partial z} - \frac{C^2}{36} \hbar^2 \theta \frac{\partial}{\partial \theta} + \frac{\gamma - 1}{6\lambda^2 \gamma} \theta^6 \right] \Psi(\theta, z) = 0, \quad (6.78)$$

where we note that the factor $1 - C^2/36$ is different from zero at least for the range of values for \mathcal{A} of our interest, i.e., $\mathcal{A} \approx 0.067$; see discussion below equation (6.69).

In order to analyse whether the BR singularity is avoided in the quantum realm by means of the DW criterion, we focus on solving the preceding equation for the wave function Ψ in the configuration space near the singularity. As we do not expect the wave function to be peaked along the classical trajectory in this regime, R and a may take completely independent values. Therefore, to consider a region close to the (quantum) BR singularity, we should assume either $a \rightarrow \infty$ or $R \rightarrow \infty$. Both choices imply $\theta \rightarrow \infty$, but in the former case z is arbitrary whereas in the latter one $z \rightarrow \infty$. Please note that the divergence of the scalar curvature can be argued to be the dominant condition, from a geometric point of view, for the occurrence of the BR singularity. Hence, we shall consider both θ and z going to infinity as the main parametrization of the BR singularity in the configuration space. Nevertheless, we highlight that the results and conclusions

presented in this section are independent of this choice and still hold for $\theta \rightarrow \infty$ and z arbitrary.

Further simplifications can be made when solving (6.78) close to the (quantum) BR. By considering the third term containing the cross partial derivatives to be subdominant when $\theta \rightarrow \infty$, the above equation can be solved using a separation ansatz for the semi-classical wave function

$$\Psi(\theta, z) = \sum_{\tilde{k}} b_{\tilde{k}} \chi_{\tilde{k}}(\theta) \varphi_{\tilde{k}}(z), \quad (6.79)$$

where $b_{\tilde{k}}$ gives the amplitude of each solution and \tilde{k} is related to the associated energy. The validity of this approximation is analysed in appendix F. Please do not confuse \tilde{k} with the modulus of the four-momentum k^μ or the spatial curvature k , which has been set to zero. Under these approximations, equation (6.78) reduces to the following system of equations⁵ [4]

$$\hbar^2 \frac{\partial^2 \varphi_{\tilde{k}}}{\partial z^2} - \tilde{k}^2 \varphi_{\tilde{k}} = 0, \quad (6.80)$$

$$\left(1 - \frac{C^2}{36}\right) \hbar^2 \theta^2 \frac{\partial^2 \chi_{\tilde{k}}}{\partial \theta^2} - \frac{C^2}{36} \hbar^2 \theta \frac{\partial \chi_{\tilde{k}}}{\partial \theta} + \left(\frac{\gamma - 1}{6\lambda^2 \gamma} \theta^6 - \tilde{k}^2\right) \chi_{\tilde{k}} = 0. \quad (6.81)$$

The former equation can be straightforwardly worked out. The solutions are

$$\varphi_{\tilde{k}}(z) = d_1 \exp\left(\frac{\sqrt{\tilde{k}^2}}{\hbar} z\right) + d_2 \exp\left(-\frac{\sqrt{\tilde{k}^2}}{\hbar} z\right), \quad (6.82)$$

being d_1 and d_2 arbitrary constants. This corresponds to either exponential or trigonometric functions on z , depending whether \tilde{k}^2 is positive or negative, respectively. On the other hand, equation (6.81) can be solved in an exact way by means of Bessel functions, cf. 9.1.53 in reference [488]. These solutions can be expressed as [4]

$$\chi_{\tilde{k}}(\theta) = \theta^{\frac{18}{36-C^2}} \left[u_1 J_\nu \left(\frac{\tilde{\lambda}}{3\hbar} \theta^3 \right) + u_2 Y_\nu \left(\frac{\tilde{\lambda}}{3\hbar} \theta^3 \right) \right], \quad (6.83)$$

where u_1 and u_2 are integration constants, J_ν and Y_ν are the Bessel functions of first and second order, respectively, and

$$\nu^2 := \frac{36}{(36 - C^2)^2} \left[1 + 4 \frac{\tilde{k}^2}{\hbar^2} \left(1 - \frac{C^2}{36} \right) \right], \quad (6.84)$$

$$\tilde{\lambda}^2 := \frac{6(\gamma - 1)}{\lambda^2 \gamma (36 - C^2)}. \quad (6.85)$$

⁵For a different approach to the asymptotic form of the wave function Ψ see reference [422].

When near the BR singularity, i.e., for large θ , the $\chi_{\tilde{k}}$ part of the wave function Ψ behaves asymptotically as [4]

$$\chi_{\tilde{k}}(\theta) \approx \sqrt{\frac{6\hbar}{\pi\tilde{\lambda}}}\theta^{-\frac{3(24-C^2)}{2(36-C^2)}} \left[\tilde{u}_1 \exp\left(i\frac{\tilde{\lambda}}{3\hbar}\theta^3\right) + \tilde{u}_2 \exp\left(-i\frac{\tilde{\lambda}}{3\hbar}\theta^3\right) \right], \quad (6.86)$$

where \tilde{u}_1 and \tilde{u}_2 now depend on \tilde{k} ; cf. 9.2.1-2 in reference [488]. Hence, the total wave function of the universe asymptotically reads [4]

$$\begin{aligned} \Psi(\theta, z) \approx & \sqrt{\frac{6\hbar}{\pi\tilde{\lambda}}}\theta^{-\frac{3(24-C^2)}{2(36-C^2)}} \sum_{\tilde{k}} b_{\tilde{k}} \left[\tilde{u}_1 \exp\left(i\frac{\tilde{\lambda}}{3\hbar}\theta^3\right) + \tilde{u}_2 \exp\left(-i\frac{\tilde{\lambda}}{3\hbar}\theta^3\right) \right] \\ & \times \left[d_1 \exp\left(\frac{\sqrt{\tilde{k}^2}}{\hbar}z\right) + d_2 \exp\left(-\frac{\sqrt{\tilde{k}^2}}{\hbar}z\right) \right], \end{aligned} \quad (6.87)$$

near the singularity. As a result, for the condition of $d_1 = 0$ when \tilde{k}^2 positive, the wave function vanishes at the BR [4, 422]. Therefore, the DW criterion is satisfied for this boundary condition. This result points towards the avoidance of this cosmological singularity in the quantum real of $f(R)$ cosmology. Nevertheless, it should be noted that by setting $d_1 = 0$ we have dismissed a subgroup of solutions to the mWDW equation as unphysical. If future investigations show the importance of these ignored solutions, then it would be concluded that the DW criterion may not always be satisfied.

6.3.3 The LR in $f(R)$ quantum cosmology

In this section, we address the quantum fate of the LR abrupt event in the framework of $f(R)$ quantum geometrodynamics. Previously, it was shown that the alternative theory of gravity given by the function (6.44) is the most general expression for a metric $f(R)$ theory of gravity which gives the same asymptotic expansion history as GR filled with phantom DE governed by equation (6.36). Moreover, since the presence of the Ei function in the term multiplying c_2 spoils the analytical inversion of $x(R)$ in equation (6.57b), which is crucial for the exact derivation of the mWDW equation (6.66), hereafter we consider $c_2 = 0$ [5]. Thus, we focus on the simple, still general, group of alternative metric $f(R)$ theories of gravity predicting the classical occurrence of a LR abrupt event given by [4, 5]

$$f(R) = c_1 \left[27\mu^4 + 150\mu^2 R - \mu(9\mu^2 + 12R)^{\frac{3}{2}} + 2R^2 \right], \quad (6.88)$$

where we recall that $\mu = \sqrt{3}\mathcal{A}/2$ and the parameter \mathcal{A} is observationally constrained to approximately $2.75 \times 10^{-28} \text{ m}^{-1}$, see table 6.2. Given the expression

for $f(R)$, the change of variables (6.57) reads

$$q = a \sqrt{\frac{2c_1 R_\star}{f_{R_\star}}} \left(75\mu^2 - 9\mu \sqrt{9\mu^2 + 12R + 2R} \right)^{\frac{1}{2}}, \quad (6.89a)$$

$$x = \frac{1}{2} \ln \left[\frac{2c_1}{f_{R_\star}} \left(75\mu^2 - 9\mu \sqrt{9\mu^2 + 12R + 2R} \right) \right], \quad (6.89b)$$

being $f_{R_\star} = 2c_1 \left(75\mu^2 - 9\mu \sqrt{9\mu^2 + 12R_\star + 2R_\star} \right)$. The definition of the constant R_\star needed for the above change of variables to be well-defined was previously discussed for the most general case; see equation (6.58). Consequently, from equations (6.39) and (6.19) it follows [5]

$$R_\star = 4\varrho_0 \left(1 + \mu \sqrt{\frac{3}{\varrho_0}} \ln 100 \right)^2 + 6\mu \sqrt{\frac{\varrho_0}{3}} \left(1 + \mu \sqrt{\frac{3}{\varrho_0}} \ln 100 \right), \quad (6.90)$$

where ϱ_0 denotes the current value of the energy density; see equation (6.4).

For the $f(R)$ model at hands, the inverse of the relation (6.89b) runs as follows [4, 5]

$$R(x) = 84\mu^2 + \frac{1}{4c_1} f_{R_\star} e^{2x} \pm 54\mu \sqrt{\frac{1}{48c_1} f_{R_\star} e^{2x} + 2\mu^2}. \quad (6.91)$$

Please note that only the positive branch is compatible with R being an increasing function of x and $R > R_\star$. Thus, we choose the positive sign in the preceding expression. The effective potential in the mWDW equation, therefore, reads [4, 5]

$$V(q, x) = -U(x)q^6, \quad (6.92)$$

where

$$\begin{aligned} U(x) = \tilde{U} \left\{ 1 + 1644 \frac{c_1 \mu^2}{f_{R_\star}} e^{-2x} + 205992 \frac{c_1^2 \mu^4}{f_{R_\star}^2} e^{-4x} \right. \\ + 36\mu e^{-x} \left(1 + 336 \frac{c_1 \mu^2}{f_{R_\star}} e^{-2x} \right) \sqrt{\frac{3c_1}{f_{R_\star}} \left(1 + 96 \frac{c_1 \mu^2}{f_{R_\star}} e^{-2x} \right)} \\ - 12\mu \sqrt{\frac{3c_1}{f_{R_\star}} e^{-x}} \left[1 + 330 \frac{c_1 \mu^2}{f_{R_\star}} e^{-2x} + 18\mu e^{-x} \sqrt{\frac{3c_1}{f_{R_\star}} \left(1 + 96 \frac{c_1 \mu^2}{f_{R_\star}} e^{-2x} \right)} \right] \\ \left. \times \left[1 + 339 \frac{c_1 \mu^2}{f_{R_\star}} e^{-2x} + 18\mu e^{-x} \sqrt{\frac{3c_1}{f_{R_\star}} \left(1 + 96 \frac{c_1 \mu^2}{f_{R_\star}} e^{-2x} \right)} \right]^{\frac{1}{2}} \right\}, \quad (6.93) \end{aligned}$$

being $\tilde{U} := f_{R_*}/(48c_1\lambda^2 R_*)$ a constant. Contrary to the previous section, a change of variables such as (6.75) will no longer be able to make the potential one-variable-dependent and, therefore, a separation ansatz such as (6.79) is not appropriate in this case. Instead, note that the $U(x)$ part of the effective potential converges very quickly to a constant value; see figure 6.1. This feature suggests an adiabatic semi-separability type ansatz for the semi-classical wave function of the universe. This is based on the so-called Born-Oppenheimer (BO) ansatz originally formulated in the context of molecular physics [496] and first introduced in the framework of quantum cosmology in references [410, 497, 498]. Furthermore, in reference [5] we have argued that the scalar curvature can be considered more fundamental from a geometrical point of view than the scale factor, justifying that the following ansatz *à la* BO should apply

$$\Psi(q, x) = \sum_{\tilde{k}} b_{\tilde{k}} \chi_{\tilde{k}}(q, x) \varphi_{\tilde{k}}(x), \quad (6.94)$$

where we recall that x depends only on R , whereas q contains both R and a , see the definitions in (6.57). Additionally, $b_{\tilde{k}}$ represents the amplitude of each solution and \tilde{k} is related to the associated energy. (As mentioned before, please do not confuse \tilde{k} with the modulus of the four-momentum k^μ or the spatial curvature k , which has been set to zero). As a result of this ansatz, the mWDW equation (6.66) becomes

$$\hbar^2 q^2 \varphi_{\tilde{k}} \frac{\partial^2 \chi_{\tilde{k}}}{\partial q^2} - \hbar^2 \varphi_{\tilde{k}} \frac{\partial^2 \chi_{\tilde{k}}}{\partial x^2} - 2\hbar^2 \frac{\partial \chi_{\tilde{k}}}{\partial x} \frac{d\varphi_{\tilde{k}}}{dx} - \hbar^2 \chi_{\tilde{k}} \frac{d^2 \varphi_{\tilde{k}}}{dx^2} + U(x) q^6 \chi_{\tilde{k}} \varphi_{\tilde{k}} = 0. \quad (6.95)$$

The contribution of the second and third terms in the above expression can be neglected by virtue of the adiabatic assumption⁶. Therefore, equation (6.95) simplifies to

$$\hbar^2 \frac{d^2 \varphi_{\tilde{k}}}{dx^2} - \tilde{k}^2 \varphi_{\tilde{k}} = 0, \quad (6.96)$$

$$\hbar^2 q^2 \frac{\partial^2 \chi_{\tilde{k}}}{\partial q^2} + [U(x) q^6 - \tilde{k}^2] \chi_{\tilde{k}} = 0. \quad (6.97)$$

The former equation can be directly solved. The solutions are exponential and trigonometric functions on x , depending on the sign of \tilde{k}^2 . These are [5]

$$\varphi_{\tilde{k}}(x) = d_1 \exp\left(\frac{\sqrt{\tilde{k}^2}}{\hbar} x\right) + d_2 \exp\left(-\frac{\sqrt{\tilde{k}^2}}{\hbar} x\right), \quad (6.98)$$

⁶The validity of this approximation is checked in appendix G.

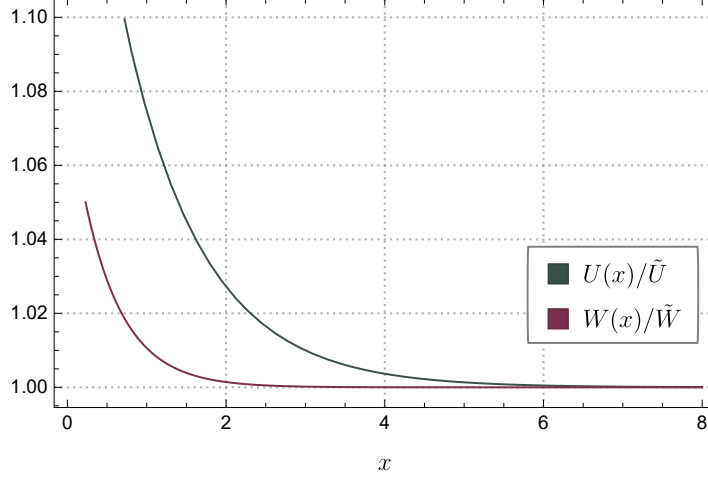


Figure 6.1: The x -dependent part of the effective potentials in the mWDW equation for the LR and the LSBR. These are the functions $U(x)$ and $W(x)$ as given in expressions (6.93) and (6.105), respectively. The value of the parameter \mathcal{A} for each case has been taken from table 6.2. As can be seen, these parts of the effective potentials quickly converge to a constant as x grows.

where d_1 and d_2 are integration constants. The solutions for $\chi_{\tilde{k}}$, on the other hand, are obtained assuming that the potential $U(x)$ behaves as a quasi-constant. Please note that this approximation is based on the fact that $U(x)$ converges very quickly to a constant value when observational constraints on the parameter \mathcal{A} are taken into account, see figure 6.1. Hence, the solutions are [5]

$$\chi_{\tilde{k}}(q, x) = \sqrt{q} \left[u_1 J_{\frac{1}{6}\sqrt{1+\frac{4\tilde{k}^2}{\hbar^2}}} \left(\frac{\sqrt{U(x)}}{3\hbar} q^3 \right) + u_2 Y_{\frac{1}{6}\sqrt{1+\frac{4\tilde{k}^2}{\hbar^2}}} \left(\frac{\sqrt{U(x)}}{3\hbar} q^3 \right) \right], \quad (6.99)$$

being u_1 and u_2 integration constants, cf. 9.1.53 of [488]. Thus, near the LR abrupt event, when both q and x diverge⁷, the resulting (semi-classical) wave function of the universe becomes [4, 5]

$$\begin{aligned} \Psi(q, x) \approx & \sqrt{\frac{6\hbar}{\pi}} \frac{1}{U(x)^{\frac{1}{4}} q} \sum_{\tilde{k}} b_{\tilde{k}} \left[\tilde{u}_1 \exp \left(i \frac{\sqrt{U(x)}}{3\hbar} q^3 \right) + \tilde{u}_2 \exp \left(-i \frac{\sqrt{U(x)}}{3\hbar} q^3 \right) \right] \\ & \times \left[d_1 \exp \left(\frac{\sqrt{\tilde{k}^2}}{\hbar} x \right) + d_2 \exp \left(-\frac{\sqrt{\tilde{k}^2}}{\hbar} x \right) \right], \quad (6.100) \end{aligned}$$

⁷This corresponds to $R \rightarrow \infty$ and a arbitrary, which was argued to be the main condition for the appearance of a curvature singularity in the quantum realm. Nevertheless, the results in this section would not change if we had considered both $a, R \rightarrow \infty$ instead.

where the integration constants \tilde{u}_1 and \tilde{u}_2 now depend on \tilde{k}^2 , see discussion in reference [5]. Since $U(x) > 0$ and tends to a constant value when x grows, the semi-classical wave function cancels as it approaches the LR abrupt event when one of the integrations constants is set to zero. This is $d_1 = 0$ when \tilde{k}^2 is positive. Hence, the DeWitt criterion can be, indeed, satisfied. This points towards the avoidance of the LR abrupt event in the quantum realm of metric $f(R)$ theories of gravity. Nevertheless, as discussed for the case of the BR in the previous section, the fulfilment of the DW criterion is conditioned to the cancellation of one of the integration constants in Ψ . Accordingly, if future investigations claim for the physical importance of the dismissed solution, then it would have to be concluded that the DW criterion may not always be satisfied.

6.3.4 The LSBR in $f(R)$ quantum cosmology

Finally, we discuss the quantum fate of the LSBR abrupt event predicted in the metric $f(R)$ theories of gravity (6.50). Moreover, following a line of reasoning similar to that presented in the previous sections, we consider $c_4 = 0$ in (6.50) as a necessary assumption to analytically obtain the corresponding mWDW equation. Therefore, we focus on the simple, still general, $f(R)$ cosmological model exhibiting a future LSBR abrupt event given by [5, 6]

$$f(R) = c_3 (9\mathcal{A}^2 - 18\mathcal{A}R + R^2), \quad (6.101)$$

where the value of \mathcal{A} is taken accordingly to table 6.2.

For the $f(R)$ gravity model (6.101), the change of variables (6.57) reads [5, 6]

$$q = a \sqrt{\frac{2c_1 R_\star}{f_{R_\star}}} (R - 9\mathcal{A})^{\frac{1}{2}}, \quad (6.102a)$$

$$x = \frac{1}{2} \ln \left[\frac{2c_1}{f_{R_\star}} (R - 9\mathcal{A}) \right], \quad (6.102b)$$

being $f_{R_\star} = 2c_1 (R_\star - 9\mathcal{A})$. Following the spirit for a physically meaningful definition of the constant R_\star given in equation (6.58), and in view of equations (6.21) and (6.47), we use [4]

$$R_\star = 4\varrho_0 + 3\mathcal{A} [1 + 4 \ln(100)], \quad (6.103)$$

where we recall that $a_\star = 100a_0$ has been set, for the sake of concreteness, as the moment in the expansion history from which we can safely assume that DE is the only relevant component of the universe; see discussion below equation (6.58).

Subsequently, the mWDW equation for the particular $f(R)$ expression considered in equation (6.101) reads [5, 6]

$$\left[\hbar^2 q^2 \frac{\partial^2}{\partial q^2} - \hbar^2 \frac{\partial^2}{\partial x^2} + W(x)q^6 \right] \Psi(q, x) = 0, \quad (6.104)$$

where $W(x)$ is given by [5, 6]

$$W(x) = \tilde{W} \left(1 + 36 \frac{c_1 \mathcal{A}}{f_{R_*}} e^{-2x} + 288 \frac{c_1^2 \mathcal{A}^2}{f_{R_*}^2} e^{-4x} \right), \quad (6.105)$$

with $\tilde{W} := f_{R_*}/(24c_1\lambda^2 R_*)$ a constant. It should be noted that (6.104) resembles the form of the corresponding mWDW equation for the LR case presented in the previous section. In fact, the $W(x)$ part of the effective potential also converges quickly to a constant value when \mathcal{A} is observationally constrained; see figure 6.1. Therefore, we consider here the very same BO approximation discussed in the previous section⁸. That is ansatz (6.94) for the semi-classical wave function

$$\Psi(q, x) = \sum_{\tilde{k}} b_{\tilde{k}} \chi_{\tilde{k}}(q, x) \varphi_{\tilde{k}}(x), \quad (6.106)$$

where $b_{\tilde{k}}$ represents the amplitude of each solution and \tilde{k} is related to the associated energy. Please avoid confusing this notation with either the modulus of the four-momentum k^μ or the spatial curvature k .

Accordingly to the results presented in the previous section, *mutatis mutandis*, the semi-classical wave function of the universe near the LSBR abrupt event is [5, 6]

$$\begin{aligned} \Psi(q, x) \approx & \sqrt{\frac{6\hbar}{\pi}} \frac{1}{W(x)^{\frac{1}{4}} q} \sum_{\tilde{k}} b_{\tilde{k}} \left[\tilde{u}_1 \exp\left(i \frac{\sqrt{W(x)}}{3\hbar} q^3\right) + \tilde{u}_2 \exp\left(-i \frac{\sqrt{W(x)}}{3\hbar} q^3\right) \right] \\ & \times \left[d_1 \exp\left(\frac{\sqrt{\tilde{k}^2}}{\hbar} x\right) + d_2 \exp\left(-\frac{\sqrt{\tilde{k}^2}}{\hbar} x\right) \right], \end{aligned} \quad (6.107)$$

⁸Please note that in reference [6] we have used a different ansatz for solving the mWDW equation (6.104). Since the exponential terms appearing in (6.105) are strongly suppressed not only by the observational value of the parameter \mathcal{A} , but also by the divergence of x , we have considered only the asymptotic value of the function $W(x)$, i.e., we have approached the effective potential in (6.104) to asymptotically depend only on the variable q . However, as argued in [5], subdominant contributions to $W(x)$ may have imprints in the shape of Ψ near the abrupt event. Those subdominant contributions can be important when comparing different wave functions that share a common asymptotic regime.

where \tilde{u}_1 and \tilde{u}_2 now depend on \tilde{k}^2 . The validity of the BO approximation in this case is verified in appendix G. Since $W(x) > 0$ and it tends to a positive constant value when x grows, the semi-classical wave function vanishes as it approaches the LSBR abrupt event when one of the integrations constants is set to zero [5, 6]. This is $d_1 = 0$ when \tilde{k}^2 is positive. Hence, the fulfilment of the DeWitt criterion points towards the avoidance of the LSBR abrupt event in the quantum realm of metric $f(R)$ theories of gravity [5, 6]. Nevertheless, as stated before, if future investigations find out the importance of the dismissed solutions, then it would be concluded that the DW criterion may not always be satisfied.

6.4 Conclusions of the chapter

The BR, LR and LSBR are cosmic curvature doomsdays predicted in some cosmological models where the super-accelerated expansion of the universe leads to the disintegration of all bound structures and, ultimately, to the tear down of space-time itself. Within the context of GR, these cosmological catastrophes are intrinsic to phantom DE models, although a phantom fluid may also induce other cosmic singularities. For a FLRW background, these events can be characterized by the behaviour of the scale factor a , the Hubble rate H and its cosmic time derivative \dot{H} near the singular fate, see table 3.1. More importantly, some of these models have been shown to be compatible with the current observational data, see, for instance, reference [137]. Therefore, our own universe may evolve towards some of these (classical) doomsdays. Nevertheless, quantum gravity effects can ultimately become significant and smooth out, or even avoid, the occurrence of these classically predicted singularities. In that sense, quantum cosmology is the natural framework for addressing the quantum fate of cosmological singularities. Among the different approaches to quantum cosmology, we have focused on the canonical quantization of the cosmological background due to DeWitt's pioneering paper [400]. In this scheme, the DW criterion can be understood as a sufficient but not necessary condition for the avoidance of a classical singularity. Thus, the classical singularity is potentially avoided if the wave function of the universe vanishes in the nearby configuration space. This criterion has been successfully applied in GR for the phantom DE models considered in section 6.1.1, which predict a classical fate *à la* BR, LR and LSBR, see references [297, 302, 304]. Consequently, this hints towards the avoidance of these cosmological doomsdays for those specific phantom DE models.

On the other hand, since the background late-time classical evolution can be equivalently described in the context of GR or within the framework of alternative theories of gravity, it is interesting to wonder whether the DW criterion is still fulfilled in the quantum realm of a different underlying theory of gravity. To

find that out, reconstruction methods can be applied to obtain the general group of alternative theories of gravity able to reproduce the same expansion history as that of a given general relativistic model. Thus, we have discussed the different $f(R)$ theories of gravity (see section 6.2) that produce the same asymptotic background expansion as the phantom DE models summarized in the preceding section 6.1.1. Consequently, these $f(R)$ models predict the classical occurrence of a BR, LR or a LSBR abrupt event. For the evaluation of the quantum fate of these classical models, we have followed the $f(R)$ quantum geometrodynamics approach introduced by Vilenkin [478], where the WDW equation is adapted for the case of $f(R)$ theories of gravity. Within this framework, the application of the DW criterion has been discussed, showing that it is possible to find semi-classical solutions to the mWDW equation (6.66) where the semi-classical wave function vanishes as the aforementioned cosmic events are approached. Therefore, as it happens when the gravitational interaction is that provided by GR, this result hints towards the avoidance of these cosmological doomsdays within the scheme of metric $f(R)$ theories of gravity [5, 6, 422].

It should be noted, however, that the validity of the wave functions obtained in this chapter is subject to the fulfilment of the conditions discussed in the appendices. Thus, for the avoidance of the BR singularity, for instance, we found our approximations to the wave function of the universe to be legitimate only for very tiny values of the parameter \mathcal{A} . It should be also noted that we have applied the quantization procedure only to some particular solutions to the reconstruction method, i.e., we have quantized just some specific $f(R)$ functions from the more general family of metric $f(R)$ gravity found to classically predict a future fate *à la* BR, LR or LSBR. Furthermore, certain boundary conditions have also been imposed when solving for Ψ to obtain vanishing solutions at the singular minisuperspace. These conditions typically involve the cancellation of one of the integration constants. Therefore, a whole subgroup of solutions to the mWDW equation has been disregarded as unphysical. If future investigations show the importance of the dismissed solutions, then it would be concluded that the DW criterion may not always be fulfilled for solutions of physical interest.

Part IV

Conclusions and appendices

7

Concluding remarks

IN this PhD dissertation we have separately considered certain type of scalar-tensor theories as fundamental frameworks for addressing questions about the late-time acceleration of the universe and the role of DE in shaping its ultimate fate. The analysed models belong to the so-called *viable* Horndeski theory and, therefore, they trivially evade the Ostrogradski ghost and predict that GWs propagate luminically. For selected models, we have explored different features related, for instance, to their background evolution, the occurrence of DE-driven singularities, the stability of cosmological perturbations and the possible resolution of classically predicted singularities within the realm of quantum cosmology.

In the first part of this thesis, we focus on the shift-symmetric version of the viable Horndeski theory, which reduces to the shift-symmetric KGB theory. The reason for considering this symmetry is two-fold. First of all, this symmetry argument naturally prevents potential-like terms for the scalar field to appear in the action. Thus, it may help to avoid reintroducing aspects of the fine-tuning problem that were originally linked to the cosmological constant. Secondly, the existence of a global symmetry leads to a (covariantly) conserved quantity which drastically reduces the complexity of the field equations. This is the shift-current J , which can be trivially employed to find a first integral of motion, see equation (4.14). In fact, the vanishing of this current with the expansion of the cosmos has been often used to discuss the future state of the system.

We start chapter 4 by arguing, however, that considering only the vanishing of J is not, in general, an exhaustive characterization of all the possible future critical states of the theory. Our approach to this issue and our findings can be summarised as follows:

- Using a dynamical systems analysis, we proposed an autonomous system which features a compact configuration space. This approach is crucial to identify equilibrium points at the boundary of the systems, otherwise such fixed points may be overlooked. For an expanding FLRW universe, we find that, in general, five different groups of critical configurations exist in these shift-symmetric scalar field theories. One of those, the group 3, strongly suggests the presence of (future) cosmological singularities. However, this ultimately depends on the underlying dynamics of the system and, therefore, on the particular KGB model under consideration.

- By investigating specific power-law examples, we found that different future attractors from a dS state exist within the physical configuration space. Specifically, we found that an evolution towards a future BR singularity is always possible for the examples at hand. Furthermore, we also identified the presence of finite size singularities, like the BF or the sudden singularity. The presence of these finite size singularities provides an excellent example of why $J = 0$ is not, as we argued at the beginning, an exhaustive characterization of all the possible future evolutions for an expanding universe in the shift-symmetric KGB theory. This is because in these models the observable universe reaches a maximum size and, therefore, the shift-current (4.14) is non-trivial on the future attractor as long as the shift-charge Q_0 is not null.
- We also identified various examples where the EOS parameter of the scalar field tends to the same value as that of the dominant matter content when evaluated on the fixed points of the model, that is, w_ϕ^{fp} matches $w_{\text{eff}}^{\text{fp}}$ when the scalar field is subdominant; see, for instance, the points \mathcal{A}_1 , \mathcal{A}_2 and \mathcal{A}_3 in tables 4.1, 4.2 and 4.3, respectively. This suggests the existence of solutions to the field equations where the scalar field mimics some of the other material components during the evolution in (at least) the nearby configuration space.

We wish to emphasise, however, that the autonomous system we have proposed is well-defined only for monotonically expanding geometries. As a result, recollapsing (turnaround) cosmologies or bounce-like events cannot be properly addressed within our current framework. Given the potential relevance of these events to cosmology, an intriguing avenue for future research would be to adapt our dynamical system approach to encompass these scenarios while preserving the compactness of the configuration space. Such an extension would undoubtedly be non-trivial, as it would require rethinking the dynamical variables we have employed (the partial energy densities) which are not suited to capture the fixed points associated with these events, if any. Equilibrium points corresponding to purely contracting FLRW models are also excluded from our analysis. Nevertheless, these can be readily incorporated into our discussion by simply reversing the direction of time in our dynamical system. Another interesting direction for future work would be a more in-depth investigation into the moment when the denominators in the auxiliary functions C_1 and C_2 vanish. As discussed in chapter 5, this may correspond to the limit $D \rightarrow 0$ within the configuration space and might indicate a pressure singularity, through which the system is unable to evolve. For the simple model proposed in section 4.3.2, we were able to identify that this moment is indeed associated with the occurrence of a BF or sudden singularity.

In chapter 5, on the other hand, we focus on the stability of cosmological perturbation in the shift-symmetric KGB theory. The main results from our dis-

cussion can be summarised as follows:

- First, we review the stability of linear scalar perturbations in the k -essence theory. In doing so, we reinterpret previously established results, demonstrating that $c_s^2 D \propto 1 + w_\phi$; see equation (5.13). This new concise expression reinforces the well-known fact, albeit from a different perspective, that violation of the NEC at the level of the associated ϕ -fluid inevitably leads to instabilities within these scalar field theories. However, the converse is not automatically true: the fulfilment of the NEC does not guarantee the stability of the theory, as both D and c_s^2 can still be negative. Ultimately, the stability in such cases depends on the specific k -essence model under consideration.
- Even though the KGB theory is well-known for allowing the possibility of a stable phantom regime, the limiting case where only the braiding function G is present performs significantly worse than k -essence in this regard. Indeed, we show that the presence of a ghost instability depends on the sign of w_ϕ ; see equation (5.18). Therefore, any model aiming to describe the current accelerated expansion (where w_ϕ must necessarily be less than $-1/3$) will inevitably encounter at least a ghost-like instability at the level of linear order scalar perturbations, if not a gradient instability as well; see figure 5.1.
- The braiding term $G \square \phi$ in the KGB action (2.21) has been shown to produce interactions between DE perturbations and GWs in a way that induces a ghost and/or gradient instability in the scalar sector when considering perturbation theory beyond linear order [286]. As previously discussed in the literature, this interaction raises significant doubts about the viability of any KGB model with a non-negligible amount of *braiding* in recent cosmic history, during which interactions with (astrophysical) GWs are expected. However, it should be noted that the original study focused primarily on the special case of the cubic Galileon (i.e., $G \propto X$). Revisiting this analysis, we identified a potential way to relax the constraints on the viable amount of *braiding* for models that deviate from a linear dependence of G on the kinetic term. Testing this idea with a power-law prescription for G revealed, however, that this approach may be futile, as the interaction between DE fluctuations and GWs persists at recent times in such models.

Our conclusions regarding the inevitability of the detrimental DE-GWs interaction are, of course, contingent upon the specific models we have explored. An interesting direction for future research would be to consider more general scenarios than the power-law functions discussed in section 5.2.3. Additionally, breaking the shift symmetry could also offer an intriguing direction for testing whether the

mechanism we proposed to mitigate the constraints on the amount of *braiding* due to this interaction might yield better results.

Another promising research line for future work would be a more detailed exploration of the connection between the stability of the linearised perturbations and the NEC within the full KGB framework. The discussion presented in the first part of chapter 5 provided us with strong intuition about the stability limits of the k -essence theory and the limiting scenario when only the function G is present. However, the picture for the complete KGB theory, when both K and G functions are non-trivial, is more complicated. While it is well-established that a stable phantom regime is possible, key questions persist: how phantom and for how long? In that sense, the precise trigger for (linear) instabilities within the full KGB set-up remains elusive.

Understanding these triggers could be of particular importance for modelling DE, especially if the DE-GWs interaction proves inevitable, as it would constrain the current level of *braiding* (characterised in α_B [194]) to remain small. In such a scenario, an intriguing question arises: what type of (stable) phenomenology, different from that of k -essence, can be modelled with a small yet non-zero amount of *braiding*?

Despite the viability concerns regarding the KGB theory discussed above, the presence of future classical singularities in the models under consideration strongly motivates a quantum analysis of their ultimate fate. This approach would involve a detailed study of the corresponding WDW equation, along with the potential application of the DW criterion. Even independently of the theory's physical viability, such an exploration may be of interest purely from the perspective of its mathematical structure, which differs significantly from that of a minimally coupled scalar field.

Shifting to a different theoretical framework for addressing the accelerated expansion of the universe, chapter 6 is entirely devoted to the classical and quantum fate of rip-like singularities and abrupt events in metric $f(R)$ theories of gravity, where we again have an additional scalar DOF with respect to GR. Our findings might be summarised as follows:

- In the framework of GR, we re-analysed the phantom EOS (2.1) in terms of the behaviour of the scale factor, the Hubble rate and its derivative. Hence, we provide a metric classification of all possible phantom futures, where we explicitly found different values for the exponent α leading to a LR or a LSBR.
- We discussed how reconstruction techniques can be employed to formulate an $f(R)$ theory of gravity with the same (future) expansion profile as that

of DE with a given EOS in GR. Within this approach, we obtain the most general $f(R)$ gravity expressions that leads to some specific LR and LSBR models.

- We solved the mWDW equation showing that it is possible to find semi-classical solutions with a vanishing wave function at the aforementioned cosmic events. Therefore, as it happens when the gravitational interaction is that provided by GR with phantom DE, this result hints towards the avoidance of these cosmological doomsdays within the scheme of metric $f(R)$ theories of gravity

The discussion presented in this chapter has also raised additional questions that should be addressed. Bound structures have been demonstrated to disintegrate before reaching either the (classical) BR singularity or the abrupt events associated with LR or LSBR scenarios. Therefore, it would be interesting to consider whether semi-classical effects may affect the disintegration of bound structures when approaching the quantum realm. In other words, while the singularity or abrupt event may be avoided within the framework of quantum cosmology, how are different bound structures impacted in such a context in the semi-classical regime? In addition to that, we should highlight that strictly speaking, the DW criterion is not a sufficient condition to guarantee the avoidance of classical singularities. To have a complete analysis, one should obtain the probability of the universe to be in those states and/or the expectation values of the relevant operators. Nonetheless, the calculation of expectation values and probability distributions are related to various open questions in quantum cosmology that still must be properly addressed in the framework of quantum geometrodynamics.

A Auxiliary functions

TAKING into account the expression for the shift-current (4.7), the scalar field equation (4.13) can be expanded as

$$A(H, X)X' + 6\epsilon\sqrt{2X}^{\frac{3}{2}}G_X H' + 3\epsilon\sqrt{2X}J = 0, \quad (\text{A.1})$$

with the function

$$A(H, X) := K_X + 2XK_{XX} + 6\epsilon\sqrt{2X}H(G_X + XG_{XX}), \quad (\text{A.2})$$

introduced for the sake of the notation. In addition, the Raychaudhuri equation (4.4) can be re-expressed as

$$HH' - 3\epsilon\sqrt{2X}G_X HX' + 9H^2 + \varrho_r + 3K = 0, \quad (\text{A.3})$$

where the Friedmann equation (4.3) has been used to eliminate ϱ_m . Thus, expressions (A.1) and (A.3) can be thought of as a system of two equations for H' and X' . Provided that this system of equations is non-degenerate, the solutions are

$$H' = -\frac{(9H^2 + \varrho_r + 3K)A + 18XG_X HJ}{6H(A + 6X^2G_X^2)}, \quad (\text{A.4})$$

$$X' = \frac{\epsilon\sqrt{2X}[(9H^2 + \varrho_r + 3K)XG_X - 3HJ]}{H(A + 6X^2G_X^2)}. \quad (\text{A.5})$$

Hence, the auxiliary functions C_1 and C_2 read

$$C_1 = -\frac{(9H^2 + \varrho_r + 3K)A + 18XG_X HJ}{6H^2(A + 6X^2G_X^2)}, \quad (\text{A.6})$$

$$C_2 = \frac{2XG_X[XG_X(9H^2 + \varrho_r + 3K) - 3HJ]}{H^2(A + 6X^2G_X^2)} - \frac{\epsilon\sqrt{2X}J}{H^2}, \quad (\text{A.7})$$

see definitions in (4.23) and (4.24), respectively. Note that these functions depend on H , X and ϱ_r but not on their time derivatives. Once $K(X)$ and $G(X)$ are specified, these functions can be fully expressed in terms of the new variables h , Ω_r and Ω_ϕ if definition (4.17) can be inverted to obtain the kinetic term X as a function on h and Ω_ϕ .

B Big rip singularity

THIS appendix is to remind the reader that a future BR singularity [88, 217] takes place when the Hubble rate is proportional to a positive power of the scale factor. Lets assume that for $a \geq a_*$, with a_* some reference scale, we have

$$H(a) \approx \mu \left(\frac{a}{a_0} \right)^p, \quad (\text{B.1})$$

being μ and p positive constant. The scale factor, then, evolves in time as

$$a(t) \approx a_0 \left[\frac{1}{\mu p (t_r - t)} \right]^{\frac{1}{p}}, \quad (\text{B.2})$$

where

$$t_r := t_* + \frac{1}{\mu p} \left(\frac{a_0}{a_*} \right)^p. \quad (\text{B.3})$$

Note that $t_r > t_*$ since μ and p are positive. Hence, the scale factor diverge at some finite future moment t_r . Similarly, the Hubble rate and its cosmic time derivative also blow-up at t_r given that

$$H(t) \approx \frac{1}{p(t_r - t)}, \quad (\text{B.4})$$

$$\dot{H}(t) \approx \frac{1}{p(t_r - t)^2}. \quad (\text{B.5})$$

Therefore, a future BR singularity [59] takes place at $t = t_r$.

C Configuration space example with a BR attractor

IN this appendix we discuss in more details the configuration space of the proxy braiding model (4.39) with $\beta = -2/5$, for which a future BR (global) attractor is present. To the best of our knowledge this was the first time that a BR singularity was discussed in the context of shift-symmetric KGB theories [3].

In figure C.1 we represent the configuration space with the corresponding fixed points. As a representative trajectory in the configuration space, we consider the one corresponding to the present values of $H_0 = 67.27 \text{ km s}^{-1} \text{ Mpc}^{-1}$, $\Omega_\phi^{(0)} = 0.68$, $\Omega_m^{(0)} = 0.32$ and $\Omega_r^{(0)} = 8.4 \times 10^{-5}$, which are consistent with the values reported in reference¹ [79]. This trajectory starts at a radiation-dominated BB singularity at the fixed point F_2 . Given that radiation dominates over matter at small scale factor, the system will never pass through D_2 . The apparent proximity of the trajectory to D_2 is, in fact, merely a visual artifact resulting from the compactification of the Hubble rate. Eventually, the system reaches the only attractor in the configuration space for an expanding universe, i.e. the equilibrium point E_2 . As discussed in section 4.3.2, this (global) attractor corresponds to a BR singularity and, therefore, E_2 is reached within a finite cosmic time. For the initial conditions under consideration, the BR singularity will occur in approximately 21 Gyr from the present state of the system [3].

Figure C.2 provides further information about the cosmic expansion history of the model. Owing to the evolution of the effective EOS parameter, w_{eff} , of the total fluid, the universe has entered the accelerated expansion phase at roughly $z \sim 0.46$. The transition from matter to scalar field dominance has occurred at approximately $z \sim 0.29$. Moreover, the scalar field has recently become phantom ($w_\phi < -1$) at redshift $z \sim 0.12$. However, the total fluid at the right-hand side of the Friedmann equation (4.3) will not exhibit phantom-like behaviour ($w_{\text{eff}} < -1$) until $z \sim -0.16$, moment at which \dot{H} will change its sign and, therefore, the Hubble rate will become an increasing function on time.

¹It should be emphasized that figures C.1 and C.2 do not represent a rigorous fit of this proxy model to cosmological data, but rather a qualitative analysis of the possible expansion history of the theory. To this aim, the data from reference [79] have been taken at face value for the numerical integration.

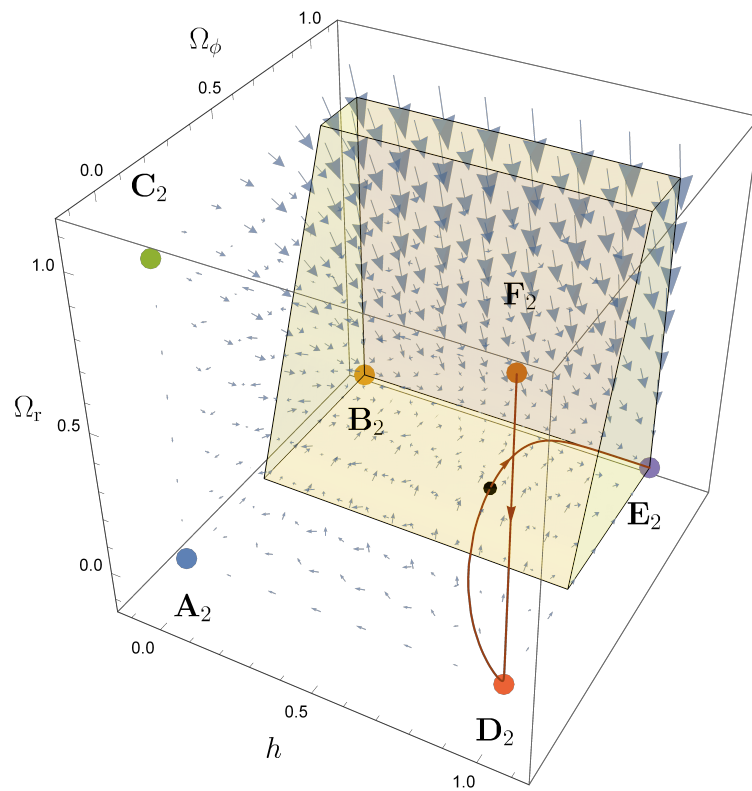


Figure C.1: Configuration space portrait of the dynamical system (4.20)-(4.22) for the proxy braiding model (4.39) with $\beta = -2/5$ (see reference [3]). The brown trajectory corresponds to the current values of $H_0 = 67.27 \text{ km s}^{-1} \text{ Mpc}^{-1}$, $\Omega_\phi^{(0)} = 0.68$, $\Omega_m^{(0)} = 0.32$ and $\Omega_r^{(0)} = 8.4 \times 10^{-5}$ [79]. The black dot on the trajectory shows the present state of the system. The yellow-shaded volume represents the region in the configuration space where the universe is accelerating. The fixed point E_2 corresponds to a BR attractor; cf. table 4.2.

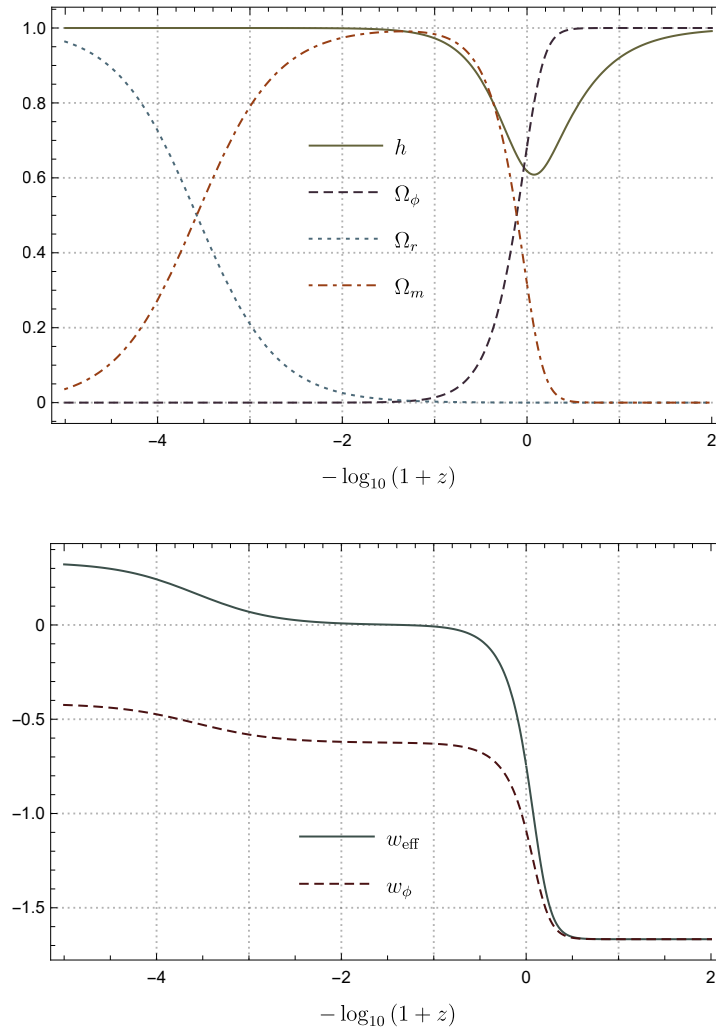


Figure C.2: Numerical integration of the dynamical system (4.20)-(4.21) for the proxy braiding model (4.39) with $\beta = -2/5$ [3]. The same initial conditions as in figure C.1 are used. Top panel: the compactified Hubble rate, h , and the partial densities Ω_i for $i = \{m, r, \phi\}$. Bottom panel: the evolution of the effective EOS parameter, w_{eff} , of the total fluid and the EOS for the scalar field, namely w_ϕ .

D Linear stability of the shift-symmetric theory

IN this appendix we discuss the possibility of satisfying simultaneously the ghost and gradient-free conditions for linear scalar perturbations given by the inequalities (5.21) and (5.24), respectively. In order to make our notation more compact, it will be useful to introduce the two following reference scales

$$\Omega^* := \frac{(3 + \Omega_r - 3\Omega_\phi)\Omega_J^B}{3(2 - \Omega_J^B)}, \quad (\text{D.1})$$

$$\bar{\Omega} := \frac{2 + \eta}{3 + \eta}(1 + w_\phi)\Omega_\phi - \frac{\Omega_J^B(2 - \Omega_J^B)}{6(3 + \eta)}, \quad (\text{D.2})$$

where Ω^* is well-defined only for $\Omega_J^B \neq 2$. The case of $\Omega_J^B = 2$ can be directly addressed using the expressions (5.21) and (5.24). We consider here the parameter η to be positive since that is the case proposed in section 5.2.2 for avoiding a GWs-induced gradient instability. Also note that the quantity $\Omega_r + 3 - 3\Omega_\phi$ is always positive¹. Hence, Ω^* is positive if $\Omega_J^B \in (0, 2)$, whereas it is negative for $\Omega_J^B < 0$ and $\Omega_J^B > 2$.

Combining the ghost and the gradient-free conditions lead to the following scenarios in which both conditions are satisfied for η non-negative:

Scenario 1 ($\Omega_J^B < 0$, $\Omega_J > \max\{(1 + w_\phi)\Omega_\phi, \Omega^*, \bar{\Omega}\}$): Both the numerator and the denominator in equation (5.21) are positive. The reference scale Ω^* is negative. Stable phantom behaviour is allowed.

Scenario 2 ($0 < \Omega_J^B < 2$, $\max\{(1 + w_\phi)\Omega_\phi, \bar{\Omega}\} < \Omega_J < \Omega^*$): The numerator and the denominator in equation (5.21) are positive. The reference scale Ω^* is also positive. Clearly, $\max\{(1 + w_\phi)\Omega_\phi, \bar{\Omega}\} < \Omega^*$ should hold for consistency. Stable phantom behaviour is allowed.

Scenario 3 ($0 < \Omega_J^B < 2$, $\max\{\Omega^*, \bar{\Omega}\} < \Omega_J < (1 + w_\phi)\Omega_\phi$): The numerator and the denominator in equation (5.21) are negative. The reference scale Ω^* is positive and, therefore, so it is Ω_J . Hence, from the upper bound for Ω_J it follows that the scalar field cannot be phantom.

¹This is because $\Omega_r + 3 - 3\Omega_\phi = 4\Omega_r + 3\Omega_m$, which is clearly positive since the energy densities of radiation and matter are non-negative.

Scenario 4 ($\Omega_J^B = 2, \Omega_J > \max\{(1 + w_\phi)\Omega_\phi, \bar{\Omega}\}$): The numerator and the denominator in equation (5.21) are positive. Note that $\bar{\Omega} > (1 + w_\phi)\Omega_\phi$ if the scalar field is phantom-like and, therefore, Ω_J should be greater than $\bar{\Omega}$. In the non-phantom regime, the lower bound for Ω_J is given by $(1 + w_\phi)\Omega_\phi$.

Scenario 5 ($\Omega_J^B > 2, \Omega_J > \max\{(1 + w_\phi)\Omega_\phi, \Omega^*, \bar{\Omega}\}$): The numerator and the denominator in equation (5.21) are positive. The reference scale Ω^* is negative. Stable phantom behaviour is allowed.

Even though the physical intuition behind each of these scenarios is not so transparent as for the marginal models studied in sections 5.1.1 and 5.1.2, their very existence is a solid proof that it is possible to have a ghost-free and gradient-free scalar perturbations at linear level (recall we consider here only the case of η non-negative) in the shift-symmetric KGB theory even when $w_\phi < -1$.

E The effective field theory of Kinetic Gravity Braiding

IN this appendix we gather useful calculations for the discussion of the KGB theory in the framework of the EFT of DE. The results here presented will be particularly important for the discussion in chapter 5. Even though in the main body of the thesis we have focussed only on the shift-symmetric case of the KGB theory, in this appendix we relax this assumption. Hence, the results here discussed are valid for the most general KGB scenario.

When applying the general EFT framework to the KGB theory given by action (2.21), the background quantities in the decomposition (2.53) read [174]

$$f = 1, \quad (\text{E.1})$$

$$c = \frac{1}{2}(\varrho_\phi + p_\phi), \quad (\text{E.2})$$

$$\Lambda = \frac{1}{2}(\varrho_\phi - p_\phi), \quad (\text{E.3})$$

with ϱ_ϕ and p_ϕ given by equations (2.23) and (2.24), respectively. Whereas the action (2.56) for the perturbations (up-to arbitrary order) reduces to [174]

$$S_{DE}^{(2)} = \frac{1}{2} \int d^4x \sqrt{-g} \left[M_2^4 (\delta g^{00})^2 - \bar{m}_1^3 \delta g^{00} \delta \mathcal{K} + \frac{1}{3} M_3^4 (\delta g^{00})^3 - \bar{m}_2^3 (\delta g^{00})^2 \delta \mathcal{K} + \dots \right], \quad (\text{E.4})$$

where the ellipses stand for quartic and higher-order terms. Here is important to note that only the mass parameters M_n^4 and \bar{m}_{n-1}^3 (for $n \geq 2$) are present for the KGB theory; cf. equation (2.56) (see also, for instance, reference [287]). Recall that these parameters are, in general, functions on the time coordinate t .

The appendix is structured as follows. In section E.1 we review the Stückelberg procedure for re-introducing explicitly the scalar field fluctuation in the EFT action (E.4). We also discuss there the expression of the Lagrangian density (5.28) describing the interaction between DE oscillations and GWs. In sections E.2, E.3 and E.4 we calculate the expressions for the mass parameters M_n^4 and \bar{m}_{n-1}^3 (for $n \geq 2$) in terms of the KGB functions and their derivatives.

E.1 Stückelberg procedure

The EFT action is written in the unitary gauge ($\delta\phi \equiv 0$) in which scalar field fluctuations are eaten in the metric perturbations. The scalar field perturbation can be reintroduced explicitly in the theory via the Stückelberg procedure. That is, by performing infinitesimal time diffeomorphism $t \rightarrow t + \pi(t, x)$ being π the scalar field fluctuations. However, in this approach π does not represent the original scalar field ϕ in the DE sector, but the perturbations encoding the scalar degree of freedom in the theory. The relevant transformations run as follows [499] (see also [286])

$$\delta g^{00} \rightarrow \delta g^{00} + 2g^{0\mu}\partial_\mu\pi + g^{\mu\nu}\partial_\mu\pi\partial_\nu\pi, \quad (\text{E.5})$$

$$\delta K \rightarrow \delta K - (1 - \dot{\pi})g^{ij}\partial_i\partial_j\pi + \frac{2}{a^2}\partial_i\pi\partial^i\dot{\pi} + \dots, \quad (\text{E.6})$$

where the former transformation is an exact relation to all order in π , whereas the latter has been expanded up-to second order in perturbations. In addition, any explicit function on time, say $m(t)$, in the EFT action will transform as

$$m(t) \rightarrow m(t + \pi) = m(t) + \dot{m}(t)\pi + \frac{1}{2}\ddot{m}(t)\pi^2 + \dots, \quad (\text{E.7})$$

where it is important to note that this transformation does not introduce any derivatives acting on π . Moreover, the volume element, $d^4x\sqrt{-g}$, or any scalar quantity, e.g. R , do not transform under the Stückelberg procedure.

After restoring full gauge invariance with the Stückelberg trick, it is convenient to move to the Newtonian gauge (5.26) for addressing the interaction between DE perturbations and GWs. We recall that this is given by [286]

$$g_{00} = -(1 + 2\Phi) \quad \text{and} \quad g_{ij} = a^2(1 - 2\Psi)(e^\gamma)_{ij}, \quad (\text{E.8})$$

where γ_{ij} is transverse and traceless; see equation (5.26). At this point we can already highlight that the operator introducing the kinetic mixing with gravity at leading order is \bar{m}_1^3 . This can be understood in an intuitive way by noting that the perturbation δg^{00} introduces a term proportional to $\dot{\pi}$ at linear order after the Stückelberg procedure, see equation (E.5). The extrinsic curvature, on the other hand, contains time derivative of the spatial metric, h_{ij} , when time diffeomorphism is fully restored [38] (see also, for instance, references [174, 500, 501]). Schematically, the product $\delta g^{00}\delta\mathcal{K}$, therefore, introduces a term proportional to $\dot{\pi}\dot{h}$ (at second order) into the Lagrangian. In the Newtonian gauge (5.26), this contribution is proportional to $\dot{\pi}\Psi$; see reference [174]. For the same reason, the functions \bar{m}_{n-1}^3 (for $n \geq 2$) will also be responsible for introducing the kinetic mixing between scalar perturbations and the GWs at higher orders.

At linear order in the perturbed equations, the Newtonian potentials can be solved as [183, 286, 440]

$$\Phi = \Psi = -\frac{\bar{m}_1^3}{2}\pi, \quad (\text{E.9})$$

where we have focussed on the sub-Hubble limit only, i.e. physical scales smaller than the Hubble horizon. The strategy for finding the Lagrangian density (5.28) consist in identifying all the contributions to cubic-order from the EFT action (E.4) after the Stückelberg procedure. The desired (cubic) contributions should also have at least two derivatives per term, where expression (E.9) can be used to substitute Φ and Ψ in terms of π . An example of such a term reads

$$\delta g^{00} \delta \mathcal{K} \supset \frac{\dot{\pi}^2}{a^2} \partial_i \partial^i \pi. \quad (\text{E.10})$$

Moreover, since the typical frequencies involved in the GWs surveys are much higher than the Hubble rate, we can further assume that time and spatial derivatives are much larger than the Hubble rate [183, 286, 440]. Under these assumptions, Lagrangian (5.27) follows after canonically normalizing the scalar and tensor fluctuations as [286]

$$\pi \rightarrow \sqrt{D} H \pi, \quad (\text{E.11})$$

$$\gamma_{ij} \rightarrow \frac{1}{\sqrt{2}} \gamma_{ij}, \quad (\text{E.12})$$

respectively, being D the ghost function (5.2).

E.2 Mass parameters for k -essence

Now, we are going to calculate the expression of the mass parameter of the free function in the covariant approach, and their derivatives. As a warm-up, we consider first the k -essence theory. In the most general scenario, the k -essence function depends on both the scalar field and its kinetic term; i.e. $K = K(\phi, X)$. (We remind the reader that we will not invoke a shift-symmetry here; thus, the results obtained in this appendix are valid for the most general case.) When perturbing this function, one may naively consider that perturbations around the background values of both ϕ and X should be taken into account. However, in the unitary gauge (defined by $\delta\phi \equiv 0$) only the perturbations of the kinetic term remains. Let the perturbed kinetic term be defined as

$$\mathcal{X} := X + \delta X, \quad (\text{E.13})$$

where X is the background value and δX the perturbation. In the unitary gauge, the perturbed kinetic term \mathcal{X} is related to the perturbed metric through

$$\mathcal{X} = -\frac{1}{2}\dot{\phi}^2 g^{00} = -Xg^{00}, \quad (\text{E.14})$$

being g^{00} the perturbed time-time component of the metric. Hence,

$$\delta X = -X\delta g^{00}, \quad (\text{E.15})$$

in the unitary gauge. Consequently, the perturbed k -essence function becomes

$$K(\phi, \mathcal{X}) \xrightarrow{\text{unitary gauge}} K(t, g^{00}), \quad (\text{E.16})$$

where we have assumed that ϕ and its kinetic term are functions of time only at the FLRW background. Note that the scalar field does not appear explicitly in the unitary gauge: it is “eaten” in the metric degrees of freedom [174, 287]. However, in order to obtain the expressions for the mass parameters in the EFT language in terms of $K(\phi, X)$ and its derivatives, it will be useful to maintain the usual covariant notation for the function K and its arguments instead of $K(t, g^{00})$ when there is no risk for confusion. Please note that this is an abuse of notation since neither ϕ nor X can appear explicitly in this gauge. They are simply functions on the time coordinate.

In this notation, the k -essence function can be expanded around its background value as

$$K(\phi, \mathcal{X}) = K(\phi, X) + \sum_{n=1}^{\infty} \frac{1}{n!} \left. \frac{\partial^n K(\phi, \mathcal{X})}{\partial \mathcal{X}^n} \right|_{\delta X=0} (\delta X)^n, \quad (\text{E.17})$$

where subscript “ $\delta X = 0$ ” denotes evaluation of the corresponding quantity at the background level. For the sake of the compactness of the notation, we will avoid writing explicitly the arguments of the function K and its derivatives appearing in the r.h.s. of the expansion, where it should be kept in mind that these expressions are always evaluated on the background. We will also omit the subscript “ $\delta X = 0$ ” in the following and express the coefficient in the expansion simply as $\partial^n K / \partial X^n$ where there is no risk for confusion. Accordingly, the above expansion can be rewritten as

$$K(\phi, \mathcal{X}) = K - XK_X - XK_X g^{00} + \sum_{n=2}^{\infty} \frac{(-X)^n}{n!} \frac{\partial^n K}{\partial X^n} (\delta g^{00})^n, \quad (\text{E.18})$$

where we have substituted $\delta X = \mathcal{X} - X$ at first order in the expansion, and used equations (E.14) and (E.15) to explicitly introduce g^{00} and δg^{00} , respectively. Comparing the above expression with equations (2.53) and (2.56), it is

straightforward to readout the contribution of the k -essence function to the EFT parameters. These are¹ [174]

$$c = XK_X, \quad (\text{E.19})$$

$$\Lambda = XK_X - K, \quad (\text{E.20})$$

$$M_n^4 = (-X)^n \frac{\partial^n K}{\partial X^n}, \quad (\text{E.21})$$

for $n \geq 2$. Therefore, the k -essence function K contributes only to the mass parameters M_n^4 at perturbation level. Since the functions \bar{m}_{n-1}^3 (for $n \geq 2$) are not present, the kinetic mixing between scalar and tensor perturbations discussed in this thesis does not occur in the k -essence theory.

E.3 Mass parameters for $G\Box\phi$

Before going to the detailed derivation of the mass parameters, it will be useful to note that

$$\begin{aligned} \int d^4x \sqrt{-g} l(t) \mathcal{K} &= \int d^4x \sqrt{-g} l(t) \nabla_\mu n^\mu \\ &= - \int d^4x \sqrt{-g} n^\mu \partial_\mu l = - \int d^4x \sqrt{-g} \sqrt{-g^{00}} \dot{l}, \end{aligned} \quad (\text{E.22})$$

up-to boundary terms and for any function $l(t)$ on time.

From the definition of the d'Alembertian operator and the slicing vector n_μ in equation (2.16), it is straightforward to check that

$$\Box\phi = -\epsilon \left(\sqrt{2X} \mathcal{K} + \frac{n^\mu}{\sqrt{2X}} \partial_\mu X \right). \quad (\text{E.23})$$

As a side note, we shall highlight from the above expression that one may consider the KGB theory as a genuine modification of gravity through a non-minimal coupling to the trace of the extrinsic curvature. To compute the EFT parameters for the braiding part of the KGB action (2.21), it will be useful to consider the following expansion in polynomials of δX [174]

$$G(\phi, \mathcal{X}) = \epsilon \sqrt{2\mathcal{X}} \sum_{m=0}^{\infty} l_m (\delta X)^m, \quad (\text{E.24})$$

¹Please note the different convention for the definition of the kinetic term used here compared to the one adopted in reference [174]. Also note that it is always possible to redefine the scalar field in a way that $\phi(t) = \sqrt{2t}$ and, therefore, the kinetic term would simply read $X = 1$ when evaluated on the background [174]. However, we will not consider such redefinition here in order to explicitly keep the kinetic term, X , in the final expressions for the EFT parameters.

where $\mathcal{X} = X + \delta X$ is the perturbed kinetic term and

$$l_m = \frac{1}{m!} \frac{\partial^m}{\partial \mathcal{X}^m} \left(\frac{G(\phi, \mathcal{X})}{\epsilon \sqrt{2\mathcal{X}}} \right) \Big|_{\delta X=0}, \quad (\text{E.25})$$

are the coefficients in the expansion evaluated on the background. Recall that we are not imposing shift-symmetry in this section. Consequently, the above coefficients depend on the background values of both the scalar field and its kinetic term. That is $l_m = l_m(\phi, X)$. Let us emphasise again that this is an abuse of notation, since neither ϕ nor its kinetic term can explicitly appear in the unitary gauge. As mentioned in the previous section, background quantities as ϕ and X are functions of time only, whereas scalar perturbations are encoded in time-time component of the metric. Hence, the perturbed braiding function, G , and the expansion coefficients, l_m , should read $G(t, g^{00})$ and $l_m(t)$ in this gauge choice, respectively. Nevertheless, this abuse of notation will be convenient, where there is no risk of confusion, for obtaining the expressions of the EFT parameters in terms of $G(\phi, X)$ and its derivatives.

Perturbing equation (E.23), and taking into account equations (E.22) and (E.24), we obtain after few integrations by parts that

$$\begin{aligned} \int d^4x \sqrt{-g} (-G \square \phi) &= \int d^4x \sqrt{-g} \left\{ - \left(\dot{X} l_0 + 2X \dot{l}_0 \right) \sqrt{-g^{00}} \right. \\ &+ \left. \sum_{n=1}^{\infty} (-X)^n \left[\left(2X l_n + \frac{2n-1}{n} l_{n-1} \right) \mathcal{K} + \left(\dot{X} l_n - \frac{\dot{l}_{n-1}}{n} \right) \sqrt{-g^{00}} \right] (\delta g^{00})^n \right\}, \end{aligned} \quad (\text{E.26})$$

up-to boundary terms; cf. with equation (86) in reference¹ [174]. The time derivative of the coefficients l_n can be simplified by noting that

$$\dot{l}_n = \dot{\phi} \frac{\partial l_n}{\partial \phi} + (n+1) \dot{X} l_{n+1}, \quad (\text{E.27})$$

where it should be kept in mind that these coefficients are evaluated on the background. Since $\mathcal{K} = 3H + \delta \mathcal{K}$, and expanding $\sqrt{-g^{00}}$ in powers of δg^{00} as

$$\sqrt{-g^{00}} = \sqrt{1 - \delta g^{00}} = 1 - \sum_{n=1}^{\infty} \lambda_n (\delta g^{00})^n, \quad (\text{E.28})$$

where

$$\lambda_n := \frac{(2n)!}{4^n (n!)^2 (2n-1)}, \quad (\text{E.29})$$

we can readout the contribution of $-G\Box\phi$ to all terms in the effective action (2.56). (Note that $G\Box\phi$ enters with a minus in the action (2.21), in contrast with the convention used in reference [174].) These are

$$c = XG_X \left(3H\dot{\phi} - \ddot{\phi} \right) - 2XG_\phi, \quad (\text{E.30})$$

$$\Lambda = XG_X \left(3H\dot{\phi} + \ddot{\phi} \right), \quad (\text{E.31})$$

$$M_n^4 = n! \left[a_n + 3Hb_n + 2\lambda_n X \left(G_\phi + G_X \ddot{\phi} \right) - \sum_{m=1}^{n-1} \lambda_m a_{n-m} \right], \quad (\text{E.32})$$

$$\bar{m}_{n-1}^3 = -2b_{n-1}, \quad (\text{E.33})$$

for $n \geq 2$, and where we have defined

$$a_n := \frac{(-1)^{n+1} \dot{\phi} X^n \partial l_{n-1}}{n \partial \phi}, \quad (\text{E.34})$$

$$b_n := (-X)^n \left(2Xl_n + \frac{2n-1}{n} l_{n-1} \right), \quad (\text{E.35})$$

with the coefficient l_n from in equation (E.25). Please note that the background parameters c and Λ , and the first order mass parameters M_2^4 and \bar{m}_1^3 were already computed, for instance, in references [174, 314] (note the different conventions used there). (See also reference [499] for a discussion on the cubic and quartic order parameters in (2.56).) Nevertheless, to the best of our knowledge, this is the first time these mass parameters are explicitly obtained in terms of the function G and its derivatives for an arbitrary order.

E.4 Mass parameters for the KGB theory

The background quantities and mass parameters for the complete KGB theory (2.21) are given by the sum of the results presented in the two previous sections. These read

$$c = XK_X + XG_X \left(3H\dot{\phi} - \ddot{\phi} \right) - 2XG_\phi, \quad (\text{E.36})$$

$$\Lambda = XK_X - K + XG_X \left(3H\dot{\phi} + \ddot{\phi} \right), \quad (\text{E.37})$$

$$M_n^4 = (-X)^n \frac{d^n K}{dX^n} + n! \left[a_n + 3Hb_n + 2\lambda_n X \left(G_\phi + G_X \ddot{\phi} \right) - \sum_{m=1}^{n-1} \lambda_m a_{n-m} \right], \quad (\text{E.38})$$

$$\bar{m}_{n-1}^3 = -2b_{n-1}, \quad (\text{E.39})$$

for $n \geq 2$. As to be expected, the combinations $c + \Lambda$ and $c - \Lambda$ (see definitions (E.2) and (E.3)) coincide with the expressions for ϱ_ϕ and p_ϕ for the non shift-symmetric KGB theory [40] (also compare with the shift-symmetric version introduced in equations (4.8) and (4.9), respectively). In addition, the leading order ($n = 2$) mass parameters read

$$M_2^4 = X^2 K_{XX} + \frac{1}{2} X G_X \left(3H\dot{\phi} + \ddot{\phi} \right) + 3H\dot{\phi} X^2 G_{XX} - X^2 G_{\phi X}, \quad (\text{E.40})$$

$$\bar{m}_1^3 = 2\dot{\phi} X G_X. \quad (\text{E.41})$$

These results coincide with those presented in the literature modulo sign conventions and numerical factors in the definition of X ; cf. with, for instance, references [174, 314]. Moreover, in accordance with the results presented in Table 2 of reference [194], note that M_2^4 is connected with the *kineticity* term α_K defined in equation (5.4) through $4M_2^4 = H^2 \alpha_K - 2c$, whereas α_B is equal to \bar{m}_1^3 (modulo sign conventions); see definition in equation (5.5).

For the discussion in section 5.2, it is also important to compute the next-to-leading order braiding operator \bar{m}_2^3 . This is

$$\bar{m}_2^3 = -\frac{1}{2} \dot{\phi} X (G_X + 2X G_{XX}), \quad (\text{E.42})$$

as can be seen from equation (E.39). Comparing this expression with that of \bar{m}_1^3 in equation (E.41), it follows that

$$4\bar{m}_2^3 = -2\dot{\phi} X G_X \left(1 + \frac{2X G_{XX}}{G_X} \right) = -\bar{m}_1^3 \left(1 + \frac{2X G_{XX}}{G_X} \right). \quad (\text{E.43})$$

Consequently, the parameter η used to measure deviations w.r.t. cubic Galileon (i.e. $G(X) \propto X$) in expression (5.32) reads

$$\eta = \frac{2X G_{XX}}{G_X}, \quad (\text{E.44})$$

which is precisely the quantity first introduced in equation (5.25).

Finally, for the shift-symmetric case of the KGB theory the function K and G depend on the kinetic term X but not on the scalar field itself. In this scenario, the expressions (E.37) and (E.38) simplify as G_ϕ vanishes. In addition, the coefficients a_n also become trivial since there is no dependence on ϕ in the shift-symmetric case; see definition (E.34). Nevertheless, the formulas for the background quantity Λ and the braiding-related parameters \bar{m}_{n-1}^3 remain absolutely the same. Thus,

the EFT parameters for the shift-symmetric KGB theory simply read

$$c = XK_X + XG_X \left(3H\dot{\phi} - \ddot{\phi} \right), \quad (\text{E.45})$$

$$\Lambda = XK_X - K + XG_X \left(3H\dot{\phi} + \ddot{\phi} \right), \quad (\text{E.46})$$

$$M_n^4 = (-X)^n \frac{d^n K}{dX^n} + n! \left(3Hb_n + 2\lambda_n XG_X \ddot{\phi} \right), \quad (\text{E.47})$$

$$\bar{m}_{n-1}^3 = -2b_{n-1}, \quad (\text{E.48})$$

for $n \geq 2$, where λ_n and b_n are defined in equations (E.29) and (E.35), respectively.

F Validity of the wave function used to describe the big rip

WHEN solving the mWDW equation near the BR singularity, we have neglected the contribution of the third term in (6.78). This approach is valid as long as the corresponding solutions satisfy

$$\begin{aligned} \frac{C}{3} \hbar^2 \theta \frac{\partial \chi_{\tilde{k}}}{\partial \theta} \frac{\partial \varphi_{\tilde{k}}}{\partial z} &\ll \left(1 - \frac{C^2}{36}\right) \hbar^2 \theta^2 \varphi_{\tilde{k}} \frac{\partial^2 \chi_{\tilde{k}}}{\partial \theta^2}, \quad \hbar^2 \chi_{\tilde{k}} \frac{\partial^2 \varphi_{\tilde{k}}}{\partial z^2}, \\ \frac{C^2}{36} \hbar^2 \theta \varphi_{\tilde{k}} \frac{\partial \chi_{\tilde{k}}}{\partial \theta}, \quad \frac{\gamma - 1}{6\lambda^2 \gamma} \theta^6 \chi_{\tilde{k}} \varphi_{\tilde{k}}. \end{aligned} \quad (\text{F.1})$$

Within this approximation, the solutions for $\chi_{\tilde{k}}$ and $\varphi_{\tilde{k}}$ are presented in equations (6.82) and (6.83). Therefore, the terms we kept in equation (6.78) are

$$\begin{aligned} \left(1 - \frac{C^2}{36}\right) \hbar^2 \theta^2 \varphi_{\tilde{k}} \frac{\partial^2 \chi_{\tilde{k}}}{\partial \theta^2} &\approx -\sqrt{\frac{6\tilde{\lambda}^3 \hbar}{\pi}} \left(1 - \frac{C^2}{36}\right) \theta^{6 - \frac{3(24-C^2)}{2(36-C^2)}} \sum_{\tilde{k}} b_{\tilde{k}} \left[\tilde{u}_1 \exp\left(i \frac{\tilde{\lambda}}{3\hbar} \theta^3\right) \right. \\ &\quad \left. + \tilde{u}_2 \exp\left(-i \frac{\tilde{\lambda}}{3\hbar} \theta^3\right) \right] \left[d_1 \exp\left(\frac{\sqrt{\tilde{k}^2}}{\hbar} z\right) + d_2 \exp\left(-\frac{\sqrt{\tilde{k}^2}}{\hbar} z\right) \right], \end{aligned} \quad (\text{F.2})$$

$$\begin{aligned} \hbar^2 \chi_{\tilde{k}} \frac{\partial^2 \varphi_{\tilde{k}}}{\partial z^2} &\approx \sqrt{\frac{6\hbar}{\pi \tilde{\lambda}}} \tilde{k}^2 \theta^{6 - \frac{3(24-C^2)}{2(36-C^2)}} \sum_{\tilde{k}} b_{\tilde{k}} \left[\tilde{u}_1 \exp\left(i \frac{\tilde{\lambda}}{3\hbar} \theta^3\right) \right. \\ &\quad \left. + \tilde{u}_2 \exp\left(-i \frac{\tilde{\lambda}}{3\hbar} \theta^3\right) \right] \left[d_1 \exp\left(\frac{\sqrt{\tilde{k}^2}}{\hbar} z\right) + d_2 \exp\left(-\frac{\sqrt{\tilde{k}^2}}{\hbar} z\right) \right], \end{aligned} \quad (\text{F.3})$$

$$\begin{aligned} \frac{C^2}{36} \hbar^2 \theta \varphi_{\tilde{k}} \frac{\partial \chi_{\tilde{k}}}{\partial \theta} &\approx \frac{C^2}{36} \sqrt{\frac{6\tilde{\lambda} \hbar^3}{\pi}} \theta^{3 - \frac{3(24-C^2)}{2(36-C^2)}} \sum_{\tilde{k}} b_{\tilde{k}} \left[\tilde{u}_1 \exp\left(i \frac{\tilde{\lambda}}{3\hbar} \theta^3\right) \right. \\ &\quad \left. - \tilde{u}_2 \exp\left(-i \frac{\tilde{\lambda}}{3\hbar} \theta^3\right) \right] \left[d_1 \exp\left(\frac{\sqrt{\tilde{k}^2}}{\hbar} z\right) + d_2 \exp\left(-\frac{\sqrt{\tilde{k}^2}}{\hbar} z\right) \right], \end{aligned} \quad (\text{F.4})$$

$$\frac{\gamma - 1}{6\lambda^2 \gamma} \theta^6 \chi_{\tilde{k}} \varphi_{\tilde{k}} \approx \frac{\gamma - 1}{6\lambda^2 \gamma} \sqrt{\frac{6\hbar}{\pi \tilde{\lambda}}} \theta^{6 - \frac{3(24-C^2)}{2(36-C^2)}} \sum_{\tilde{k}} b_{\tilde{k}} \left[\tilde{u}_1 \exp\left(i \frac{\tilde{\lambda}}{3\hbar} \theta^3\right) \right]$$

$$+ \tilde{u}_2 \exp\left(-i \frac{\tilde{\lambda}}{3\hbar} \theta^3\right) \left] \left[d_1 \exp\left(\frac{\sqrt{\tilde{k}^2}}{\hbar} z\right) + d_2 \exp\left(-\frac{\sqrt{\tilde{k}^2}}{\hbar} z\right) \right]. \quad (\text{F.5})$$

However, the terms that we have neglected behave asymptotically as

$$\begin{aligned} \frac{C}{3} \hbar^2 \theta \frac{\partial \chi_{\tilde{k}}}{\partial \theta} \frac{\partial \varphi_{\tilde{k}}}{\partial z} &\approx i \sqrt{\frac{6\tilde{\lambda}\tilde{k}^2}{\pi\hbar}} \frac{C\hbar}{3} \theta^{3-\frac{3(24-C^2)}{2(36-C^2)}} \sum_{\tilde{k}} b_{\tilde{k}} \left[\tilde{u}_1 \exp\left(i \frac{\tilde{\lambda}}{3\hbar} \theta^3\right) - \tilde{u}_2 \exp\left(-i \frac{\tilde{\lambda}}{3\hbar} \theta^3\right) \right] \\ &\times \left[d_1 \exp\left(\frac{\sqrt{\tilde{k}^2}}{\hbar} z\right) - d_2 \exp\left(-\frac{\sqrt{\tilde{k}^2}}{\hbar} z\right) \right]. \quad (\text{F.6}) \end{aligned}$$

We recall that the integration constants d_1 must be set to zero to fulfil the DW criterion at the BR when \tilde{k}^2 positive. Thus, to obtain the compliance region of the performed approximation we compare the largest of the neglected terms with the smallest of the saved ones. This is the ratio

$$\epsilon = \left| \frac{\frac{B}{3} \hbar^2 \theta \partial_\theta \chi_{\tilde{k}} \partial_z \varphi_{\tilde{k}}}{\hbar^2 \chi_{\tilde{k}} \partial_z^2 \varphi_{\tilde{k}}} \right| \approx \frac{2}{3|\tilde{k}|} \frac{\gamma - 2}{\gamma - 1} \tilde{\lambda} \theta^3. \quad (\text{F.7})$$

Please note that the bigger \tilde{k} is, the smaller the ratio ϵ becomes. This ratio also keeps below one if $\gamma - 2$ is sufficiently small to compensate the increase of the variable θ towards the BR singularity. Therefore, for $\gamma \approx 2$, this approximation is valid throughout the semi-classical regime towards the BR singularity, where θ increases but not sufficiently rapidly to compensate the small value of $\gamma - 2$. In the expression (6.34) for the metric $f(R)$ theory of gravity predicting the BR singularity, this would correspond to having a small parameter \mathcal{A} and $c_+ = 0$, since γ_+ diverge at $A \rightarrow 0$. Consequently, this argument would favour small deviations from the Λ CDM model. It is worth noting that the values estimated for \mathcal{A} in reference [137] are not small enough to ensure $\epsilon \ll 1$; however smaller values for \mathcal{A} are compatible with the fits claimed in other references (see, for example, references [78, 79, 120]). Thus, we consider this approximation to Ψ valid for the appropriate γ value.

Additionally note that in this appendix, we have enhanced the discussion on the viability of the performed approximations for Ψ originally presented in reference [422], where the authors have focused only on the particular case of $\tilde{k} = 0$ when addressing the validity of the wave function there found.

G

Validity of the Born-Oppenheimer approximation

DURING the application of the BO-type ansatz (6.94) performed in sections 6.3.3 and 6.3.4, we have considered that $\chi_{\tilde{k}}(q, x)$ depends adiabatically on x . Therefore, we have neglected the contribution of some parts in their corresponding mWDW equations. This approach is valid as long as the corresponding solutions satisfy

$$\hbar^2 \varphi_{\tilde{k}} \frac{\partial^2 \chi_{\tilde{k}}}{\partial x^2}, 2\hbar^2 \frac{\partial \chi_{\tilde{k}}}{\partial x} \frac{d\varphi_{\tilde{k}}}{dx} \ll \hbar^2 q^2 \varphi_{\tilde{k}} \frac{\partial^2 \chi_{\tilde{k}}}{\partial q^2}, \hbar^2 \chi_{\tilde{k}} \frac{d^2 \varphi_{\tilde{k}}}{dx^2}, U(x) q^6 \chi_{\tilde{k}} \varphi_{\tilde{k}}. \quad (\text{G.1})$$

As a result of this approximation, the solutions for $\varphi_{\tilde{k}}$ and $\chi_{\tilde{k}}$ obtained for the case of the LR abrupt event are presented in equations (6.96) and (6.97), respectively (see also reference [5]). Then, the terms we keep in (6.95) read

$$\begin{aligned} \hbar^2 q^2 \varphi_{\tilde{k}} \frac{\partial^2 \chi_{\tilde{k}}}{\partial q^2} &\approx -U(x) q^6 \chi_{\tilde{k}} \varphi_{\tilde{k}} \approx -\sqrt{\frac{6\hbar}{\pi}} U(x)^{\frac{3}{4}} q^5 \left[\tilde{u}_1 \exp\left(i \frac{\sqrt{U(x)}}{3\hbar} q^3\right) \right. \\ &\quad \left. + \tilde{u}_2 \exp\left(-i \frac{\sqrt{U(x)}}{3\hbar} q^3\right) \right] \left[d_1 \exp\left(\frac{\sqrt{\tilde{k}^2}}{\hbar} x\right) + d_2 \exp\left(-\frac{\sqrt{\tilde{k}^2}}{\hbar} x\right) \right], \end{aligned} \quad (\text{G.2})$$

$$\begin{aligned} \hbar^2 \chi_{\tilde{k}} \frac{d^2 \varphi_{\tilde{k}}}{dx^2} &\approx \sqrt{\frac{6\hbar}{\pi}} \frac{\tilde{k}^2}{U(x)^{\frac{1}{4}} q} \left[\tilde{u}_1 \exp\left(i \frac{\sqrt{U(x)}}{3\hbar} q^3\right) + \tilde{u}_2 \exp\left(-i \frac{\sqrt{U(x)}}{3\hbar} q^3\right) \right] \\ &\quad \times \left[d_1 \exp\left(\frac{\sqrt{\tilde{k}^2}}{\hbar} x\right) + d_2 \exp\left(-\frac{\sqrt{\tilde{k}^2}}{\hbar} x\right) \right]. \end{aligned} \quad (\text{G.3})$$

However, the neglected terms behave asymptotically as

$$\begin{aligned} \hbar^2 \varphi_{\tilde{k}} \frac{\partial^2 \chi_{\tilde{k}}}{\partial x^2} &\approx -\frac{1}{36} \sqrt{\frac{6\hbar}{\pi}} \frac{U'(x)^2}{U(x)^{\frac{5}{4}}} q^5 \left[\tilde{u}_1 \exp\left(i \frac{\sqrt{U(x)}}{3\hbar} q^3\right) + \tilde{u}_2 \exp\left(-i \frac{\sqrt{U(x)}}{3\hbar} q^3\right) \right] \\ &\quad \times \left[d_1 \exp\left(\frac{\sqrt{\tilde{k}^2}}{\hbar} x\right) + d_2 \exp\left(-\frac{\sqrt{\tilde{k}^2}}{\hbar} x\right) \right], \quad (\text{G.4}) \\ 2\hbar^2 \frac{\partial \chi_{\tilde{k}}}{\partial x} \frac{d\varphi_{\tilde{k}}}{dx} &\approx \frac{i}{3} \sqrt{\frac{6\hbar \tilde{k}^2}{\pi}} \frac{U'(x)}{U(x)^{\frac{3}{4}}} q^2 \left[\tilde{u}_1 \exp\left(i \frac{\sqrt{U(x)}}{3\hbar} q^3\right) - \tilde{u}_2 \exp\left(-i \frac{\sqrt{U(x)}}{3\hbar} q^3\right) \right] \end{aligned}$$

$$\times \left[d_1 \exp\left(\frac{\sqrt{\tilde{k}^2}}{\hbar}x\right) - d_2 \exp\left(-\frac{\sqrt{\tilde{k}^2}}{\hbar}x\right) \right]. \quad (\text{G.5})$$

Please note that for \tilde{k}^2 positive, the constants d_1 must be zero to have a vanishing wave function at the LR. Thus, the validity of the BO approximation can be verified comparing the largest of the neglected terms with the smallest of the saved ones. This is the ratio ε ,

$$\varepsilon = \left| \frac{\hbar^2 \varphi_{\tilde{k}} \partial_x^2 \chi_{\tilde{k}}}{\hbar^2 \chi_{\tilde{k}} \partial_x^2 \varphi_{\tilde{k}}} \right|. \quad (\text{G.6})$$

For the case of the LR abrupt event analyzed in section 6.3.3 that ratio reads

$$\varepsilon \approx \frac{U'(x)^2}{U(x)} \frac{q^6}{36|\tilde{k}^2|}. \quad (\text{G.7})$$

Consequently, the semi-classical approximation for the wave function Ψ is valid as long as $\varepsilon \ll 1$. To evaluate this condition, note that

$$\frac{U'(x)^2}{U(x)} \approx 36 \frac{\mu^2}{\lambda^2 R_\star} e^{-2x} \left[1 + \frac{40}{3} \sqrt{\frac{3c_1}{f_{R_\star}}} \mu e^{-x} + \frac{832}{3} \frac{c_1 \mu^2}{f_{R_\star}} e^{-2x} + \mathcal{O}(e^{-3x}) \right], \quad (\text{G.8})$$

when μ is observationally constrained, see Table 6.2. Thus, in the configuration space near the LR cosmic event, we have

$$\varepsilon \approx \frac{\mu^2}{\lambda^2 R_\star |\tilde{k}^2|} e^{-2x} q^6, \quad (\text{G.9})$$

where both q and x are large. Finally, $\varepsilon \ll 1$ near the LR if \tilde{k} is large and/or μ , which depends on \mathcal{A} , is sufficiently small. Please note that small values for μ corresponds, in fact, to the observationally preferred situation [137]. (We recall that \mathcal{A} is of order 10^{-28} m^{-1} when observationally constrained, see table 6.2). Therefore, when the parameters of the theory are observationally constrained, the approximation is valid throughout the semi-classical regime towards the LR abrupt event; where the variables q and x increase but not sufficiently rapidly to compensate the small value of μ^2 . Hence, for the purpose of the present work, i.e., to analyse the fulfilment of the DW criterion in the configuration space close to the LR, this (semi-classical) approximation is valid.

On the other hand, for the verification of the validity of the BO approximation performed in section 6.3.4, $U(x)$ must be exchanged for $W(x)$ in the preceding formulas. Therefore, considering the expression for $W(x)$ given in (6.105), the ratio ε becomes

$$\varepsilon \approx \frac{W'(x)^2}{W(x)} \frac{q^6}{36|\tilde{k}^2|} \approx \frac{6c_1 \mathcal{A}^2}{\lambda^2 R_\star f_{R_\star} |\tilde{k}^2|} e^{-4x} q^6, \quad (\text{G.10})$$

where the bigger \tilde{k} is, the smaller the ratio ε becomes. Following the same line of reasoning as that presented before, this ratio keeps below one since the parameter \mathcal{A} for the LSBR is of order 10^{-54} m^{-2} , see table 6.2. Therefore, the BO approximation applied in section 6.3.4 is valid throughout the semi-classical regime towards the LSBR abrupt event.

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