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Features of the primordial Universe in $f(R)$-gravity as viewed in the Jordan frame

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Abstract
We analyze some features of the primordial Universe as viewed in the Jordan frame formulation of the $f(R)$-gravity when the potential term is negligible. We start formulating the Hamiltonian picture using the three-metric determinant as a basic variable and we outline that its conjugated momentum appears linearly only in the scalar constraint. We construct the formalism to characterize the dynamics of a generic inhomogeneous cosmological model and specialize it to describe behaviors of the Bianchi Universes, both on a classical and a quantum regime. We demonstrate that, when the potential term of the additional scalar mode is negligible near to the initial singularity, the Bianchi IX cosmology is no longer affected by the chaotic behavior, typical in the vacuum of the Einsteinian dynamics. In fact, the presence of the Kasner stability region and its attractive character are properly characterized. Finally, we investigate the canonical quantization of the Bianchi I model, using as time variable the non-minimally coupled scalar field and showing that the existence of a conserved current is outlined for the corresponding Wheeler–DeWitt equation. The behavior of a localized wave-packet for the isotropic Universe is also evolved, demonstrating that the singularity is still present in this revised quantum dynamics.

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(Some figures may appear in colour only in the online journal)

1. Introduction

The standard cosmological model [1], which provides a consistent and probed general picture of the Universe thermal history, at least after a post-inflationary temperature (but also the inflationary model is a reliable theoretical framework with observational favorable indications) is entirely based on the standard Einsteinian formulation of the gravitational field (also the standard model of elementary particles has a fundamental role). However, it is a well-known fact that at very primordial instants (say pre-inflationary age) its nature can be more complicated than the simple isotropic model, and additional effects from modified and quantum gravity can become important [2–5].

The most natural generalization of the isotropic Robertson geometry is provided by the Bianchi classification [3, 6]. In particular, the Bianchi type VIII and IX cosmological models (the most general allowed by the homogeneity constraint) have an Einsteinian chaotic dynamics [7–9], which constitutes a valuable prototype for the asymptotic behavior to the singularity of the generic inhomogeneous Universe (no space symmetries are imposed) [3, 10, 11].

Furthermore, it must be noted that, while the kinematic structure of general relativity (GR), namely its covariant nature, expressed via the tensor language is a solid theoretical construction, the Einstein equations are not very general in their derivation. In fact, Einsteinian dynamics is fixed by the Einstein–Hilbert scalar action, which is the only one respecting the assumptions of the Lovelock uniqueness theorem: the action is diffeomorphism-invariant; it leads to second-order field equations for the metric; four-dimensionality; no fields other than the metric enter the gravitational action [12–15]. Among the possible restatements of the gravitational dynamics, it stands out for its simplicity and its capability to explain phenomena like dark matter and dark energy overall, the so-called $f(R)$ model, whose Lagrangian is a function of the Ricci scalar. The interest for this model relies also on the possibility to restate the $f(R)$ model in terms of a scalar–tensor formulation, in which a scalar field is non-minimally coupled to standard gravity in the so-called *Jordan frame* or minimally coupled to it in the so-called Einstein frame [13, 14, 16].

It is worth noting that, as well known [13], a simplification of the dynamical picture for the scalar–tensor $f(R)$-gravity can be obtained passing to the so-called Einsteinian frame. This configuration can be achieved by a conformal rescaling of the metric tensor, which provides the scalar degree of freedom in the form of a scalar field minimally-coupled to gravity. On a classical level, these two representations of the $f(R)$ model are equivalent. However, the real physical degrees of freedom naturally live in the Jordan frame, while the Einsteinian one, being based on a non-physical transformation, must be regarded as a valuable technical tool only. When studying the cosmological implementation of an $f(R)$ model, the Jordan frame appears privileged as the Universe dynamics unavoidably explore the Planckian era, where the gravitational setting must be quantized. In the quantum sector, the equivalence between the Jordan and the Einsteinian framework is no longer well-established. On a quantum level, we are legitimated to quantize only the physical degrees of freedom of the scalar–tensor theory and, in this respect, the use of the Jordan frame is mandatory. Since we intend to construct a cosmological setting of the scalar–tensor formulation of the $f(R)$ model, able to cover, in principle, the whole Universe history, we will consider, in what follows, the Jordan frame as the natural arena for our study (see in particular the quantum analysis developed in part VI).

We finally observe that the canonical quantization of the gravitational field is also an open problem in the $f(R)$ model, calling attention as in the case of ordinary Einsteinian gravity. In fact, the idea that the corrections to the Einstein–Hilbert action must be relevant when the Universe density overcome the nuclear density and, more in general, near enough to the initial singularity, must be conjugated with the idea that, in the same limit, at Planckian scales, the quantum dynamics of the gravitational field is a mandatory description. In this paper, we provide a general discussion of the primordial Universe in the $f(R)$ formulation of the gravitational field, as viewed in the Jordan frame, facing both symmetric and generic models, as well as both classical and quantum effects; for related topics see [17–20]. We start by re-analyzing the study presented in [21], in which the Hamiltonian formulation of the $f(R)$ gravitational dynamics in the Jordan frame is developed. In particular, we introduce a representation of the three-metric tensor in which the three-determinant is isolated, like in the original analysis in [22]. Thus, we outline that the conjugate momentum to the three-determinant enters linearly only in the gravitational Hamiltonian. Considerations on the structure of the corresponding Wheeler–DeWitt (WDW) equation are developed, clarifying how it seems to resemble the morphology of a Schrödinger functional equation (although non-local) than a Klein–Gordon (KG) functional equation as in standard gravity [2] with respect to the choice of the three-determinant as the time-like variable. On the basis of the general formulation above traced, we consider the formulation of a generic cosmological model in the Jordan frame, generalizing similar studies developed in Einsteinian gravity, see [23–27]. Then, we specialize this scheme to the symmetric case of the homogeneous but anisotropic Bianchi universes, for which we construct the generic Hamiltonian picture, then focusing attention on the Bianchi I and Bianchi IX models. Here we provide a detailed analysis of the Bianchi IX Universe, demonstrating that, as far as the potential term of the non-minimally coupled scalar field (depending on the form of f) is negligible, the chaos of the standard gravitational dynamics in vacuum is removed. We outline the existence of the so-called *generalized Kasner solution* and, via a numerical analysis, we show its attractivity during the system evolution. Finally, we face the treatment of quantum features of the $f(R)$-gravity in the Jordan frame, by implementing the Dirac canonical method to the restated Hamiltonian constraints. We pay attention to the Bianchi I cosmological model, constructing a conserved current for the associated WDW equation. The construction of an evolutive wave packet is limited to the isotropic case only, being that, if the non-minimally coupled scalar field potential is negligible, the singularity still appears in the generalized quantum gravity framework of the Jordan frame, having chosen such a field as the system internal time. The comparison with the case of the standard Einsteinian isotropic quantum Universe in the presence of a minimally coupled scalar field as a matter clock is finally provided.

The manuscript is organized as follows: in section 2 we present the $f(R)$ theories of gravity in the so-called *Jordan frame*. We also introduce the $f(R)$ Hamiltonian formalism and then we quantize it using the Dirac scheme.

In section 3 we deal with the formalism of the generic cosmological problem of the $f(R)$ theories in the Jordan frame.

In section 4 we analyze the features of classical $f(R)$ cosmology. We derive Kasner solutions and then we use them to determine the conditions for which the scalar field potential is negligible. We also perform an analysis of the Bianchi IX cosmology showing the attractivity of the stability region.

In section 5 we perform a critical study on the canonical quantization of the Bianchi I model and of the homogeneous and Friedmann-Lemaître-Robertson-Walker Universe (FLRW) in the case of the $f(R)$ theories of gravity in the Jordan frame. In particular, using the non-minimally coupled scalar field as a quantum time, we carry out an analysis on the quantum dynamics of the FLRW model, and finally, we make a comparison with the case of a minimally coupled external scalar field in GR.

In section 6 concluding remarks follow.

2. *f*(*R*)-gravity

Einstein's theory of GR represents the current classical theory of gravity. Its geometrical and tensorial structure determines the kinematics of the gravitational field in a very consistent formulation, but its dynamics admits a wide class of different proposals. In fact, as stated in the introduction section, the Einstein–Hilbert Lagrangian $\mathcal{L}_{\mathrm{EH}} = R$ is only the most simple proposal.

2.1. The Jordan frame

A more general formulation of the gravitational field dynamics consists in the replacement of the Ricci scalar by a generic function $f(R)$. In the $f(R)$ theories of gravity the corresponding action of the gravitational field takes the form:

$$S = \frac{1}{2k}\int \mathrm{d}^4x\sqrt{-g}f(R) + S_M\big(g_{\mu\nu},\psi\big), \tag{1}$$

where $k = 8\pi Gc^{-4}$ and $-g$ is the positive determinant of the metric tensor $g_{\mu\nu}$ and ψ denotes a generic matter field. In this way, a new geometric degree of freedom is included in the theory (the function f), which induces different field equations [13]. Variation $\delta_{g_{\mu\nu}}S = 0$ with respect to the metric $g_{\mu\nu}$ gives the following set of fourth-order covariant field equations

$$f'(R)R_{\mu\nu} - \frac{1}{2}f(R)g_{\mu\nu} - \left[\nabla_\mu\nabla_\mu - g_{\mu\nu}\Box\right]f'(R) = kT_{\mu\nu}, \tag{2}$$

where $f'(R) = \frac{\mathrm{d}f}{\mathrm{d}R}$ and $\Box = g^{\sigma\rho}\nabla_\sigma\nabla_\rho$ is the d'Alembert operator in curved manifolds.

The action (1) can take the form

$$S = \frac{1}{2k}\int \mathrm{d}^4x\sqrt{-g}[\phi R - V(\phi)] + S_M\big(g_{\mu\nu},\psi\big). \tag{3}$$

This is the Jordan frame representation of the action of a Brans–Dicke theory with Brans–Dicke parameter $\omega_0 = 0$. Action (3) is also known as the $f(R)$ gravitational action in the Jordan frame. It is the scalar–tensor equivalent representation of the action (1), expressed through a non-minimal coupling between a scalar field (ϕ) and the curvature (R).

2.2. Jordan frame Hamiltonian of f(R)-gravity

The Arnowitt-Desner-Misner (ADM) action of $f(R)$-gravity in the Jordan frame (with $k \equiv 1$) is the following

$$S_{\mathrm{JF}}^{\mathrm{ADM}}\big(h_{ij},N,N^i,\phi\big) = \int_{\mathbb{R}\times\Sigma}\mathrm{d}t\,\mathrm{d}^3x\,N\sqrt{h}\left[\frac{\phi}{2}\left({}_TK\cdot{}_TK - \frac{2}{3}K^2 + {}^3R\right) - \frac{1}{2}V(\phi) + \right.$$
$$\left. -\frac{K}{N}\left(\dot{\phi} - N^i\partial_i\phi\right) + \frac{1}{N}\partial_i\phi\partial^iN\right], \tag{4}$$

where ${}^3R\left(h_{ij},\partial_l h_{ij},\partial_m\partial_l h_{ij}\right)$ is the Ricci three-scalar, ${}_TK_{ij}=\left(K_{ij}-\frac{1}{3}h_{ij}K\right)$; ${}_TK\cdot{}_TK={}_TK_{ij\,T}K^{ij}$ and $h=\det\left(h_{ij}\right)$.

In analogy with the articles [21, 28], by performing a Legendre transformation, we obtain the following Hamiltonian density

$$\begin{aligned}\mathcal{H}_{\mathrm{JF}}^{\mathrm{ADM}}&=N\left[\frac{2}{\sqrt{h}}\left(\frac{{}_Tp\cdot{}_Tp}{\phi}+\frac{1}{6}\phi\pi_\phi^2-\frac{1}{3}p\pi_\phi\right)+\right.\\&\left.+\frac{\sqrt{h}}{2}\left(V(\phi)-\phi\,{}^3R+2D_iD^i\phi\right)\right]+N^i\left[\pi_\phi\partial_i\phi-2D^jp_{ij}\right]=\\&=N\mathcal{H}_{g,\mathrm{JF}}+N^i\mathcal{H}_{i,\mathrm{JF}}^g,\end{aligned}\tag{5}$$

where we have highlighted respectively the so-called *superHamiltonian* $\mathcal{H}_{g,\mathrm{JF}}$ and *supermomentum* $\mathcal{H}_{i,\mathrm{JF}}^g$ which represent the two secondary constraints of the theory as we can see from Hamilton's equations

$$\begin{cases}\delta_N S_{\mathrm{JF}}^{\mathrm{ADM}}=0\rightarrow-\dfrac{\partial\mathcal{H}_{\mathrm{JF}}^{\mathrm{ADM}}}{\partial N}\rightarrow\mathcal{H}_{g,\mathrm{JF}}=0,\\[2mm]\delta_{N^i}S_{\mathrm{JF}}^{\mathrm{ADM}}=0\rightarrow-\dfrac{\partial\mathcal{H}_{\mathrm{JF}}^{\mathrm{ADM}}}{\partial N^i}\rightarrow\mathcal{H}_{i,\mathrm{JF}}^g=0.\end{cases}\tag{6}$$

The prefix *super*, conceived by Wheeler, indicates that the configurational space of canonical gravity is the space of all Riemannian three-metrics Riem(Σ) modulo the spatial diffeomorphisms group Diff(Σ) on the slicing surface Σ. Explicitly

$$\{h_{ij}\}=\frac{\mathrm{Riem}(\Sigma)}{\mathrm{Diff}(\Sigma)}.\tag{7}$$

This is the space of all three-geometries and it is known as the *Wheeler superspace*: the ∞-dimensional functional space of all the equivalence classes of three-metrics $h_{ij}\left(t,x^l\right)$ linked together by three-diffeomorphisms.

As discussed in [21] the constraints $\mathcal{H}_{g,\mathrm{JF}}$ and $\mathcal{H}_{i,\mathrm{JF}}^g$ comprise a first class constraint similar to GR as:

$$\begin{aligned}\{\mathcal{H}_{i,\mathrm{JF}}^g(N^i),\mathcal{H}_{i,\mathrm{JF}}^g(N^{i'})\}&=\mathcal{H}_{i,\mathrm{JF}}^g([N^i,N^{i'}]),\\\{\mathcal{H}_{i,\mathrm{JF}}^g(N^i),\mathcal{H}_{g,\mathrm{JF}}(N)\}&=\mathcal{H}_{g,\mathrm{JF}}(\mathcal{L}_{N^i}N),\\\{\mathcal{H}_{g,\mathrm{JF}}(N),\mathcal{H}_{g,\mathrm{JF}}(M)\}&=\mathcal{H}_{i,\mathrm{JF}}^g(ND^aM-MD^aN),\end{aligned}\tag{8}$$

where $\mathcal{L}$ is the Lie derivative.

A confirmation of the closure of this algebra is also provided by the independent gauge covariant analysis in [29, 30]. It is there demonstrated that the basic mode of the linearized $f(R)$ theory, in the Jordan frame, are only three. A scalar mode is added to the two standard tensorial representations. This result confirms the first-class character of the obtained constraints. By a simple counting of the theory degree of freedom, we have 22 phase space variables and the usual eight first-class constraints of the standard gravity, which eliminate 16 degrees of freedom. It is straightforward that we arrive at the right number of six phase space degrees of freedom for the considered modified gravity.

2.3. Wheeler–De Witt equation

The canonical theory of gravity, also in his $f(R)$ extension, can be written as a dynamical system subjected to first-class constraints with a Dirac algebra. In *Wheeler's superspace*, the dynamics of the gravitational field is generated by imposing the *superHamiltonian* constraint, which leads to the WDW equation. It is well known that in GR the WDW equation can be seen as a KG equation with a varying mass. By defining the new set of variables $\{\xi, u_{ij}\}$

$$\begin{cases} \xi = h^{\frac{1}{4}}, \\ h_{ij} = \xi^{\frac{4}{3}} u_{ij}, \quad u = \det(u_{ij}) = 1, \end{cases} \tag{9}$$

and imposing the canonical transformation

$$\pi_\xi \partial_t \xi + \pi^{ij} \partial_t u_{ij} = p^{ij} \partial_t h_{ij}, \tag{10}$$

we can immediately obtain the WDW–KG-like equation in GR

$$\begin{aligned} \hat{\mathcal{H}}_g |\Psi\rangle &= \left[\frac{2k}{\xi^2} \left(\hat{\pi}^{ij} \hat{\pi}^{lm} u_{il} u_{jm} - \frac{3}{32} \xi^2 \hat{\pi}_\xi^2 \right) - \frac{\sqrt{h}}{2k} {}^3R \right] |\Psi\rangle = \\ &= 2k\hbar^2 \left[\frac{3}{32} \frac{\delta^2}{\delta\xi^2} - \frac{1}{\xi^2} u_{il} u_{jm} \frac{\delta^2}{\delta u_{ij} \delta u_{lm}} + \right. \\ &\quad \left. - \frac{\xi^2}{(2k\hbar)^2} {}^3R \right] \Psi\big(\xi, \{u_{ij}\}\big) = 0, \end{aligned} \tag{11}$$

where the variable ξ is timelike (internal time), while the variables u_{ij} are spacelike. We now review the corresponding formalism in the case of the $f(R)$ theory in the Jordan frame. Following the same procedure described above, the *superHamiltonian* $\mathcal{H}_{g,\mathrm{JF}}$ in the new canonical variables $\{\xi, \pi_\xi; u_{ij}, \pi_{ij}; \phi, \pi_\phi\}$ takes the form

$$\begin{aligned} \mathcal{H}_{g,\mathrm{JF}} = \frac{2}{\xi^2} \bigg[& \frac{1}{\phi} \big(\pi^{ij} \pi^{lm} u_{il} u_{jm} \big) + \frac{1}{6} \phi \pi_\phi^2 - \frac{1}{4} \xi \pi_\xi \pi_\phi + \\ & + \frac{\xi^4}{4} \big(V(\phi) - \phi\, {}^3R\big(\xi, u_{ij}, \partial\xi, \partial u_{ij}\big) + 2 D_i D^i \phi \big) \bigg]. \end{aligned} \tag{12}$$

Applying the Dirac quantization, we obtain the WDW–KG-like equation in the Jordan frame

$$\begin{aligned} \hat{\mathcal{H}}_{g,\mathrm{JF}} |\Psi\rangle = \frac{2}{\xi^2} \bigg[& \frac{1}{\phi} \big(\hat{\pi}^{ij} \hat{\pi}^{lm} u_{il} u_{jm} \big) + \frac{1}{6} \phi \hat{\pi}_\phi^2 - \frac{1}{4} \xi \hat{\pi}_\xi \hat{\pi}_\phi + \\ & + \frac{\xi^4}{4} \big(V(\phi) - \phi\, {}^3R + 2 D_i D^i \phi \big) \bigg] |\Psi\rangle, \\ 0 = 2\hbar^2 \bigg[& - \frac{1}{\xi^2 \phi} u_{il} u_{jm} \frac{\delta^2}{\delta u_{ij} \delta u_{lm}} - \frac{\phi}{6\xi^2} \frac{\delta^2}{\delta\phi^2} + \frac{1}{4\xi} \frac{\delta^2}{\delta\xi \delta\phi} + \\ & + \frac{\xi^2}{4\hbar^2} \big(V(\phi) - \phi\, {}^3R + 2 D_i D^i \phi \big) \bigg] \Psi\big(\xi, \{u_{ij}\}, \phi\big). \end{aligned} \tag{13}$$

We immediately notice that we cannot identify a d'Alembert operator in the equation, so it is not straightforward to identify a phase space variable playing the role of a quantum time in the theory. One result that deserves to be taken seriously, is the linearity of the equation with respect to the conjugate momentum π_ξ. Differently from the case of GR, the equation (13) is linear in π_ξ. This makes the WDW equation in the Jordan frame conceptually more similar to a Schrödinger-like equation, in which ξ would be the timelike variable. There are, however, substantial differences between the equation (13) and a Schrödinger one, such as the functional nature and the undefined role of variables $\{\xi, \phi\}$ as spacelike or timelike variables of the theory. In fact, there is a non-trivial coupling between the variables $\{\xi, \phi\}$, which is expressed in the third term containing mixed partial derivatives. It is also evident that, even if we choose ξ or ϕ as a quantum timelike variable, we will have to face the impossibility of performing a frequency separation procedure. This critical feature is due to the presence of the potential term $V(\phi) - \phi^3 R + 2D_i D^i \phi$ which depends on $\{\xi, \phi\}$ and their derivatives.

3. The generic cosmological problem in the Jordan frame

The generic cosmological problem represents the Hamiltonian formalism of gravity for an inhomogeneous space. In what follow we outline the main results in the canonical formalism of the generic cosmological problem in the JF.

3.1. Hamiltonian formulation in a general framework

Using the triadic formalism, the three-metric associated with a generic inhomogeneous space can be written as

$$h_{ij}(t, x^k) = \eta_{ab}(t, x^k) e_i^a(t, x^k) e_j^b(t, x^k), \tag{14}$$

where η_{ab} is its triadic representation and $a = 1, 2, 3$ are the SU(2) indices. The corresponding line element is

$$\mathrm{d}s^2 = -N\,\mathrm{d}t^2 + h_{ij}(t, x^k)\left(\mathrm{d}x^i + N^i\,\mathrm{d}t\right)\left(\mathrm{d}x^j + N^j\,\mathrm{d}t\right),$$

where $N = N(t, x^k)$ and $N^i = N^i(t, x^k)$.

We can define a generic set of three-vectors on the hypersurfaces Σ_t^3 of the ADM foliation as

$$e_i^a(t, x^k) = O_b^a(x^k)\partial_i y^b(t, x^k), \tag{15}$$

where y^b denotes three scalar functions and O_b^a is a SO(3) matrix such that $O_b^a O_a^c = \delta_b^c$. This definition of the three-vectors e_i^a, allows us to rewrite the three-metric tensor h_{ij} as

$$\begin{aligned} h_{ij}(t, x^k) &= \sum_a \mathrm{e}^{q_a(t,x^k)} e_i^a(t, x^k) e_j^a(t, x^k) = \\ &= \sum_a \mathrm{e}^{q_a(t,x^k)} O_b^a(x^k)\partial_i y^b(t, x^k) O_c^a(x^k)\partial_i y^c(t, x^k), \end{aligned} \tag{16}$$

where $q_a(t, x^k) = \ln\left(a^2(t, x^k), b^2(t, x^k), c^2(t, x^k)\right)$ denotes the three inhomogeneous cosmological scale factors.

Imposing the canonical transformation $\left(h_{ij}, p^{ij}\right) \to (q_a, p_a; y_a, \pi_a)$

$$p^{ij}\partial_t h_{ij} = \sum_a p_a \partial_t q_a + \sum_a \pi_a \partial_t y_a, \tag{17}$$

we obtain the *superHamiltonian* $\mathscr{H}_{g,\mathrm{JF}}$ and the *supermomentum* $\mathscr{H}^{g}_{i,\mathrm{JF}}$ in the new generic framework

$$\mathscr{H}_{g,\mathrm{JF}} = \frac{2}{\sqrt{h}}\left(\frac{\sum_a p_a^2 - \frac{1}{3}\left(\sum_a p_a\right)^2}{\phi} + \frac{1}{6}\phi\pi_\phi^2 - \frac{1}{3}\sum_a p_a\pi_\phi\right) + \\ + \frac{\sqrt{h}}{2}\left(V(\phi) - \phi^3 R + 2D_iD^i\phi\right), \tag{18}$$

$$\mathscr{H}^{g}_{i,\mathrm{JF}} = \pi_\phi\partial_i\phi + \pi_a\partial_i y^a + p_a\partial_i q^a + 2p_a\left(O^{-1}\right)^b_{\ a}\partial_i O^a_b. \tag{19}$$

3.2. The generic cosmological problem in Misner-like variables

Let us introduce the Misner-like variables as $\left\{\alpha(t,x^k), \beta_\pm(t,x^k)\right\}$ via the transformation

$$\begin{cases} q_1(t,x^k) = \left(\alpha(t,x^k) + \beta_+(t,x^k) + \sqrt{3}\beta_-(t,x^k)\right), \\ q_2(t,x^k) = \left(\alpha(t,x^k) + \beta_+(t,x^k) - \sqrt{3}\beta_-(t,x^k)\right), \\ q_3(t,x^k) = \left(\alpha(t,x^k) - 2\beta_+(t,x^k)\right). \end{cases} \tag{20}$$

Imposing the canonical condition $(q_a, p_a) \to (\alpha, p_\alpha; \beta_\pm, p_\pm)$

$$p_\alpha\dot{\alpha} + p_+\dot{\beta}_+ + p_-\dot{\beta}_- = \sum_a p_a\partial_t q_a, \tag{21}$$

we can rewrite the $f(R)$ *superHamiltonian* (18) of the generic cosmological problem in Misner-like variables

$$\mathscr{H}_{g,\mathrm{JF}} == \frac{2\,\mathrm{e}^{-\frac{3}{2}\alpha}}{\mathbf{v}}\left[\frac{1}{6\phi}\left(p_+^2 + p_-^2\right) + \frac{1}{6}\pi_\phi^2\phi - \frac{1}{3}p_\alpha\pi_\phi + U(\alpha,\beta_\pm,\phi)\right], \tag{22}$$

where $U(\alpha,\beta_\pm,\phi) = \frac{\mathbf{v}^2}{4}\mathrm{e}^{3\alpha}\left(V(\phi) - \phi^3R + 2D_iD^i\phi\right)$ and $\mathbf{v}(x^l) = \det\left(e^a_i\right)$.

It is clear that, differently from the case in GR [3] where the *superHamiltonian* takes the form

$$\mathcal{H}_g = \frac{2\,\mathrm{e}^{-\frac{3}{2}\alpha}}{\mathbf{v}}\left(-p_\alpha^2 + p_+^2 + p_-^2 + U(\alpha,\beta_\pm)\right), \tag{23}$$

in the case of the $f(R)$ theories in the Jordan frame, we lost the pseudo-Riemannian structure. It is also evident that the equation (22) is the classical counterpart in the cosmological context of the WDW quantum-gravitational equation (13). Therefore, the same considerations about the problem of identifying a time variable apply. As we have already done, we highlight the linearity of the equation with respect to the conjugated momentum p_α and, therefore, the formal analogy between the equation (22) and a Schrödinger-like equation, once one assigns to α the role of the timelike variable of the theory. The presence of a potential term still does not allow the construction of a Hilbert space for physical quantum states.

4. Classical *f*(*R*) cosmology

When we use the term classical cosmology we refer to the description of the Universe using the tools provided by GR and, in this case, the equivalence with Brans–Dicke theory of $f(R)$ models. Our purpose is to analyze the Bianchi IX model, which is the prototype of the generic cosmological solution, in the Jordan frame and try to solve an already known issues of this model in standard GR: its chaotic behavior as we are going through the cosmological singularity. In order to achieve this result we need to follow some intermediate steps: recall some interesting properties of the Bianchi IX cosmology in standard GR, find a solution for the Bianchi I model, i.e. the Kasner solutions, and use these solutions to discuss some properties of the potential terms. We want to define a class of $f(R)$ theory for which we can neglect the term $V(\phi)$ in a way that the solutions became independent from the specific functional form of the theory.

About the assumption of neglecting the potential term of the scalar mode, it is justified *a priori* because of the presence of a volume factor $e^{3\alpha}$ which vanishes towards the initial singularity. However, only *a posteriori*, we can select those $f(R)$ Lagrangians for which the considered assumption holds, as discussed above in detail.

Then we discuss the properties of the potential term of the Bianchi IX model and try to find a region, in the space of parameters that describes the Kasner solutions, which removes the chaos. Finally, we will discuss the properties of our cosmological model, studying the dynamical features of the bounces that characterized the Bianchi IX model.

4.1. Bianchi IX cosmology in GR

The Bianchi models are a class of cosmologies that obey the homogeneity constraint but not the isotropy constraint. The relevance of the dynamics of Bianchi models consists in the role these geometries could have played in a very primordial Universe, before the inflation phase. For a quantum discussion on the Bianchi IX model see [31, 32]. We will focus our attention on the Bianchi IX model because we are looking for the most general cosmology allowed by the homogeneity constraint, since we do not have any clue to the need for specific symmetries and because it also admits the isotropic limit. We would like to present some properties of the Bianchi IX model in standard GR which will be useful for our further analysis.

We start with the line element of a general Bianchi model [2]:

$$ds^2 = -N^2(t)dt^2 + a^2(t)(\omega^l)^2 + b^2(t)(\omega^m)^2 + c^2(t)(\omega^n)^2. \tag{24}$$

In order to discuss the most important properties of the Bianchi models we use the *Misner variables* introduced in (20).

The choice of these variables allow us to separate the isotropic contribution, related to the variables α i.e. the logarithm of the Universe's volume, from the two degrees of anisotropy related to $\beta_\pm$. The *Misner variables* make the kinetic part of the Hamiltonian diagonal [4]. Adopting the coordinate $\alpha, \beta_\pm$ the *super-Hamiltonian* constraint, in standard GR, takes the form:

$$\mathcal{H}_B = -p_\alpha^2 + p_+^2 + p_-^2 + V_B(\alpha, \beta_\pm), \tag{25}$$

where V_B denotes a potential term, different for each Bianchi model and due to the spatial curvature and α seem to be the right time-like variable of the system.

Writing down the potential term for the Bianchi IX model we obtain:

$$\begin{aligned}2V_{\mathrm{IX}} = &\left(\mathrm{e}^{4\alpha+4\beta_{+}+4\sqrt{3}\beta_{-}} + \mathrm{e}^{4\alpha+4\beta_{+}-4\sqrt{3}\beta_{-}} + \mathrm{e}^{4\alpha-8\beta_{+}}\right)+\\ &-2\left(\mathrm{e}^{4\alpha+4\beta_{+}} + \mathrm{e}^{4\alpha-3\beta_{+}+2\sqrt{3}\beta_{-}} + \mathrm{e}^{4\alpha-2\beta_{+}-2\sqrt{3}\beta_{-}}\right).\end{aligned} \tag{26}$$

The first parenthesis dominates as we are going through the cosmological singularity, placed at $\alpha \to -\infty$, and the potential term is reduced to an infinite well with the form of an equilateral curvilinear triangle.

Far from the potential well, we can find the equations of motion by neglecting the potential term. These solutions are known as *Kasner solutions* for the so-called Bianchi I model ($V_{\mathrm{B}} = 0$).

The Hamiltonian constraint (25) can then be solved with respect to p_α [33] as:

$$p_\alpha = -h_\alpha = -\sqrt{p_+^2 + p_-^2}. \tag{27}$$

Using the Hamilton's equation we can find $\beta_\pm$ as functions of α:

$$\frac{\mathrm{d}\beta_\pm}{\mathrm{d}\alpha} = \frac{p_\pm}{p_\alpha} = \text{const}, \tag{28}$$

with $\left(\frac{\partial\beta_+}{\partial\alpha}\right)^2 + \left(\frac{\partial\beta_-}{\partial\alpha}\right)^2 = 1$.

The chaotic behavior of the Bianchi IX model in standard GR is a well known problem and it means that the vacuum Bianchi IX classical evolution is constituted by an infinite series of Kasner regimes (free motions of the point-Universe), associated with continuous scatterings against the infinite potential walls [34, 35].

Since the Bianchi IX model is not integrable [36], the scattering dynamics can be characterized deriving a function which maps the solutions before a bounce into the solutions after the bounce.

The ADM–Hamiltonian of the system can be rewritten as:

$$\mathcal{H}_{\mathrm{IX}} = \sqrt{p_+^2 + p_-^2 + \frac{1}{2}\exp\left(4\alpha - 8\beta_+\right)}, \tag{29}$$

where we included only one wall thanks to the symmetry of the potential. The Hamiltonian $\mathcal{H}_{\mathrm{IX}}$ is independent from β_- and so p_- is a constant of motion. Another constant can be found comparing p'_+ and H'_{IX}, so we can define a new constant of motion as: $c = 1/2p_+ + \mathcal{H}_{\mathrm{IX}}$.

These two constant of motion allow us to find the value of β'_+ and β'_- after the bounce as function of their value before. Since $\left(\frac{\partial\beta_+}{\partial\alpha}\right)^2 + \left(\frac{\partial\beta_-}{\partial\alpha}\right)^2 = 1$ we can parameterize $\beta'_- = \sin\,\theta$ and $\beta'_+ = \cos\,\theta$.

The constancy of p_- and c gives us, using (28)

$$\begin{aligned}\mathcal{H}^{\mathrm{i}}_{\mathrm{IX}}\,\sin\,\theta_{\mathrm{i}} =&\mathcal{H}^{\mathrm{f}}_{\mathrm{IX}}\,\sin\,\theta_{\mathrm{f}},\\ \mathcal{H}^{\mathrm{i}}_{\mathrm{IX}}\left(-1/2\,\cos\,\theta_{\mathrm{i}}+1\right) =&\mathcal{H}^{\mathrm{f}}_{\mathrm{IX}}\left(+1/2\,\cos\,\theta_{\mathrm{f}}+1\right).\end{aligned} \tag{30}$$

These can be combined to find an equation for θ_{f} as function of θ_{i},

$$\sin\,\theta_{\mathrm{f}} - \sin\,\theta_{\mathrm{i}} = \frac{1}{2}\sin(\theta_{\mathrm{f}} + \theta_{\mathrm{i}}), \tag{31}$$

which is sufficient for our purpose.

4.2. Kasner-like solutions in f(R)-gravity

The Bianchi I Universe corresponds to set $V_{\mathrm{B}}(\alpha, \beta_{\pm}) = 0$, since the structure constants of the isometry group are all zero. Strictly speaking, we are assuming also the potential $V(\phi)$ to be negligible. This assumption can be supported in relation to the inflation theory, for which during the Planck era the inflation field ([3, 37]) is a non-interacting field (for an alternative paradigm about the power-law inflation in the $f(R)$ gravity see [38, 39]). The conditions under which the potential of the $f(R)$ theory is negligible will be discussed later. The *superHamiltonian* (22) becomes

$$\mathcal{H}_{\mathrm{I,JF}} = \frac{2\,\mathrm{e}^{-\frac{3}{2}\alpha}}{\mathbf{v}}\left[\frac{1}{6\phi}\left(p_+^2 + p_-^2\right) + \frac{1}{6}\pi_\phi^2\phi - \frac{1}{3}p_\alpha\pi_\phi\right]. \tag{32}$$

In the framework of Bianchi models, it is easy to recognize the coincidence between the set of variables emerging from the ADM reduction method and the Misner variables. In particular, the anisotropies of the Universe $\beta_{\pm}$ represent the two physical degrees of freedom of Einstenian gravity, the variable α represents an embedding degree of freedom and the variable ϕ is a massive mode. Solving classically the *superHamiltonian* constraint (32) with respect to the conjugate momentum π_ϕ, we get the following quadratic equation:

$$\pi_\phi^2 - \frac{2p_\alpha}{\phi}\pi_\phi + \frac{\left(p_+^2 + p_-^2\right)}{\phi^2} = 0, \tag{33}$$

which admits the solutions

$$\pi_{\phi\,1,2} = \frac{p_\alpha}{\phi} \pm \frac{1}{\phi}\sqrt{p_\alpha^2 - p_+^2 - p_-^2} = -h_{\phi\,1,2}, \tag{34}$$

where in the last equality we highlighted the role of h_ϕ as the new Hamiltonian which regulates the dynamics with respect to the time variable ϕ.

The next step in the procedure consists in the imposition of the so-called time gauge which sets the lapse function N

$$\dot{\phi} = N\frac{\partial\mathcal{H}_{\mathrm{BM\,I,JF}}}{\partial\pi_\phi} = \frac{2N\,\mathrm{e}^{-\frac{3}{2}\alpha}}{3\mathbf{v}}\left(\phi\pi_\phi - p_\alpha\right) = 1, \tag{35}$$

$$N = N_{\mathrm{ADM}} = \frac{3\mathbf{v}\,\mathrm{e}^{\frac{3}{2}\alpha}}{2\left(\phi\pi_\phi - p_\alpha\right)}. \tag{36}$$

Since N is always positive, we obtain the condition $\phi\pi_\phi > p_\alpha$ which constrains the choice of the positive sign in equation (34).

From the Hamilton's equations

$$\begin{cases} \dfrac{\partial\alpha}{\partial\phi} = \dfrac{\partial h_\phi}{\partial p_\alpha} = -\dfrac{1}{\phi}\left(1 + \dfrac{p_\alpha}{\sqrt{p_\alpha^2 - p_+^2 - p_-^2}}\right), \\ \dfrac{\partial p_\alpha}{\partial\phi} = -\dfrac{\partial h_\phi}{\partial\alpha} = 0, \end{cases} \tag{37}$$

we can derive the equation of motion

$$\alpha(\phi) = -K\,\ln(\phi) + \alpha_0, \tag{38}$$

where we can set $\alpha_0 = 0$ by choosing the initial condition $\alpha(1) = 0$ and where K is a constant of motion defined as:

$$K = 1 + \frac{p_\alpha}{\sqrt{p_\alpha^2 - p_+^2 - p_-^2}}. \tag{39}$$

Since the Misner variable α is related to the volume of the Universe, the constant K must always be real. Consequently, we must impose the relation:

$$p_\alpha^2 > p_+^2 + p_-^2, \tag{40}$$

which constrains the value of $|K| > 1$.

The Hamilton equations takes the following form: $\mathrm{d}\beta_\pm/\mathrm{d}\phi = \partial h_\phi/\partial p_\pm$ and, since the Hamiltonian does not depend on the coordinates, the momenta are constant.

We can express the *Misner coordinates* as function of the scalar field:

$$\begin{aligned} \alpha &= -\left(1 + \frac{p_\alpha}{\sqrt{p_\alpha^2 - p_+^2 - p_-^2}}\right) \ln\,\phi, \\ \beta_\pm &= \left(\frac{p_\pm}{\sqrt{p_\alpha^2 - p_+^2 - p_-^2}}\right) \ln\,\phi. \end{aligned} \tag{41}$$

By dividing between $\beta_\pm(\phi)$ and $\alpha(\phi)$ we can find:

$$\beta_\pm(\alpha) = \frac{p_\pm}{p_\alpha \pm \sqrt{p_\alpha^2 - p_+^2 - p_-^2}} \cdot \alpha. \tag{42}$$

4.3. Potential term of f(R) theory

We want to deal with the most general scenario, without fixing the functional form of the theory. As the model we are analyzing is important only in a pre-inflation scenario, we are interested in the limit $\alpha \to -\infty$ and so we want that the potential term of ϕ in the Hamiltonian of the system vanishes as we are going to the cosmological singularity. So we can work with a class of theories, that obeys to this constraint, instead to deal with a specific theory with a specific functional form of the potential. In order to achieve our goal we will use the *Kasner solutions* found in the previous section and then we will discuss the functional form with the dominant diverging term which admits the limit we are looking for. Finally, we will define a concrete constraint of the functional form of the potential of the $f(R)$ theory.

We have to rewrite the *Kasner solutions* because we are interested in ϕ as a function of α. The Kasner solution (equation (41)) gives us $\alpha(\phi)$ that can be easily inverted in order to find:

$$\phi(\alpha) = \mathrm{e}^{-\frac{\alpha}{K}}. \tag{43}$$

We can assume that $V(\phi) \propto \phi^n$ as the limit form of the potential, because potentials that diverges faster than this are forbidden by the condition chosen on the potential.

With this choice of the potential we have:

$$\mathrm{e}^{3\alpha} V(\phi) \propto \mathrm{e}^{3\alpha}\, \mathrm{e}^{-n\alpha/K} = \mathrm{e}^{(3-n/K)\alpha}, \tag{44}$$

we have to study the sign of $3 - n/K$ because it must be positive in order to have a vanishing potential. We will now calculate the maximum n that respects the condition

$$n < 3\left(1 + \frac{p_\alpha}{\sqrt{p_\alpha^2 - p_+^2 - p_-^2}}\right). \tag{45}$$

The function of the momenta is strictly increasing and his maximum and minimum value are defined by its limits, respectively to $\pm\infty$:

$$-1 < \frac{p_\alpha}{\sqrt{p_\alpha^2 - p_+^2 - p_-^2}} < 1, \tag{46}$$

and so the value of K is also limited between 0 and 2.

Since we are interested to the maximum value of n, given $K = 2$ we find:

$$n_{\mathrm{MAX}} = 6. \tag{47}$$

For all $f(R)$ theories, leaving to a potential term which diverges slower than ϕ^6 the present and following analysis hold.

The form of the function f, due to a polynomial form of the potential $V(\phi)$, can be derived using the following differential equation:

$$f''(R)[R - V'(f'(R))] = 0. \tag{48}$$

Substituting a polynomial potential we obtain the following form of the function:

$$f(R) = (n-1)\left(\frac{R}{n}\right)^{\frac{n}{n-1}}, \tag{49}$$

so we can fix $n \in (1, 6]$.

Imposing $f(R) = R + (n-1)\left(\frac{R}{n}\right)^{\frac{n}{n-1}}$ the potential term $V(\phi)$ takes the following form:

$$V(\phi) = (\phi - 1)^n. \tag{50}$$

It is straightforward that for low curvatures, since $n/(n-1) > 1$, GR is recovered.

We observe that, for $n = 1$ a singular behavior of the obtained $f(R)$ model emerges (49) and this suggests to exclude this value in a physical formulation of the model. However, in principle, we can consider a potential term for the non-minimally couple scalar field, having the form

$$V(\phi) = \sum_{n=0}^{6} c_n \phi^n. \tag{51}$$

For such a general choice, actually to be thought as a Taylor expansion of the potential, an analytical expression for the corresponding $f(R)$ expression can not be found (for generic constants c_n), but it is natural to expect a resolution of the singularity discussed above, even when $n = 1$ is included in the development.

We observe that, in the early Universe, the scalar field $\phi(t)$ has its own dynamics and the cosmological gravitational field significantly deviates from the Einsteinian picture, while in the late Universe, near the minimum of its potential $\phi \simeq 0$, we recover Einsteinian gravity for $a_0 \neq 0$ or also a cosmological constant term.

4.4. Chaotic behavior of the Bianchi IX potential

We have already seen that the dynamics of the Bianchi IX model is completely determined by its potential. The form of the potential, in its asymptotic form, is a wall with a triangular symmetry but in a $f(R)$ theory it is multiplied by the scalar field ϕ. This feature gives us the chance to remove the chaotic behavior of this model, characterized by oscillations from one Kasner solution to another. We are looking for a region, in the space of parameters that characterized the Kasner solutions, that ensures us that the potential term will vanish as we are going to the cosmological singularity. We analyze the role of scalar field using the method of consistent potential (MCP), i.e. we assume that the approach to the singularity is asymptotically velocity term dominated [40]. If this is true, the model approaches closely to a Kasner solution. The *superHamiltonian* constraint takes the form:

$$\mathcal{H}_{\mathrm{IX,JF}} = \mathcal{H}_{\mathrm{k}} + \mathcal{H}_{\mathrm{v}}, \tag{52}$$

where $\mathcal{H}_{\mathrm{k}}$ is the kinetic term and $\mathcal{H}_{\mathrm{v}}$ stands as

$$\begin{aligned} 2\mathcal{H}_{\mathrm{v}} = \phi\, \mathrm{e}^{2\alpha}\Big\{ &\Big(\mathrm{e}^{2\beta_+ + 2\sqrt{3}\beta_-} + \mathrm{e}^{2\beta_+ - 2\sqrt{3}\beta_-} + \mathrm{e}^{-4\beta_+}\Big) \\ &- 2\Big(\mathrm{e}^{2\beta_+} + \mathrm{e}^{\beta_+ + \sqrt{3}\beta_-} + \mathrm{e}^{-\beta_+ - \sqrt{3}\beta_-}\Big)\Big\} + \mathrm{e}^{3\alpha}V(\phi). \end{aligned} \tag{53}$$

In these variables, the singularity occurs as $\alpha \to -\infty$, and as we have discussed in the previous section $\mathrm{e}^{3\alpha}V(\phi) \to 0$ going to the singularity, so we shall ignore this term. The MCP will be used in order to define a *Kasner stability region* in which the characteristic oscillation of the Mixmaster Universe are suppressed after a given sequence. The MCP requires to assume $\mathcal{H}_{\mathrm{IX,JF}} = \mathcal{H}_{\mathrm{k}}$. Variation of this Hamiltonian yields equations with the solution obtained in equation (41) which we are going to express as function of α

$$\begin{aligned} \beta_\pm &= \beta'_\pm \alpha, \\ \phi &= \mathrm{e}^{-\frac{\alpha}{K}}, \end{aligned} \tag{54}$$

where K is defined in equation (39) and $\beta'_\pm$ are defined as

$$\beta'_\pm = \frac{p_\pm}{p_\alpha + \sqrt{p_\alpha^2 - p_+^2 - p_-^2}}. \tag{55}$$

The minisuperspace potential is dominated by the first three terms of rhs of equation (53) so

$$2\mathcal{H}_{\mathrm{v}} \approx \phi \mathrm{e}^{2\alpha}\Big(\mathrm{e}^{2\beta_+ + 2\sqrt{3}\beta_-} + \mathrm{e}^{+2\beta_+ - 2\sqrt{3}\beta_-} + \mathrm{e}^{-4\beta_+}\Big), \tag{56}$$

we can write K as a function of β'_+ and β'_- considering that

$$\beta'^2_+ + \beta'^2_- = \frac{p_+^2 + p_-^2}{\Big(p_\alpha + \sqrt{p_\alpha^2 - p_+^2 - p_-^2}\Big)^2},$$

and find $p_+^2 + p_-^2$ as function of β'^2_+, β'^2_- and, inserting it into the definition of K, we can write:

$$\frac{1}{2K} = \frac{\beta'^2_+ + \beta'^2_- - 1}{4\beta'^2_+ + 4\beta'^2_-}. \tag{57}$$

Substitution of (55) and (57) into (56), yields to:

$$\mathcal{H}_{\rm v} \approx \exp\left\{2\alpha\left(1+\beta'_{+}+\sqrt{3}\beta'_{-}-\frac{\beta'^2_{+}+\beta'^2_{-}-1}{4\beta'^2_{+}+4\beta'^2_{-}}\right)\right. + \exp\left\{2\alpha\left(1+\beta'_{+}-\sqrt{3}\beta'_{-}-\frac{\beta'^2_{+}+\beta'^2_{-}-1}{4\beta'^2_{+}+4\beta'^2_{-}}\right)\right\} + \exp\left\{2\alpha\left(1-2\beta'_{+}-\frac{\beta'^2_{+}+\beta'^2_{-}-1}{4\beta'^2_{+}+4\beta'^2_{-}}\right)\right\}. \tag{58}$$

We are looking for the values of β_+ and β_- which makes all the terms going to zero as $\alpha \to -\infty$. In order to achieve our purpose we had to request that all the three terms inside round brackets to be positive.

With the help of the software *Mathematica* we have solved the three inequalities to find the values of β_+ and β_- which can make all the three exponential to vanish at the same time. The stability region is the blue region shown in figure 1.

We want to check if actual the *Kasner stability region* is an attractor for the Mixmaster dynamics. First of all, we shall remember that, near the singularity, the matter and radiation density terms are negligible because the dynamics of the Universe is dominated by the curvature term due to the geometry of the space-time. The potential term of the Bianchi IX cosmology depends on the variable α and this feature complicates the dynamics with respect to the *Kasner solution*, generating in principle a chaotic evolution. The vacuum Bianchi IX dynamics is constituted by an infinite series of Kasner regimes, associated with the continuous scatterings against the infinite potential walls. The purpose of this chapter is to verify if, thanks to the additional degree of freedom introduced by the choice of $f(R)$ framework, we are led to remove the chaotic behavior. We have already find a region, in the space (β_+, β_-) of the parameters that describe the Kasner solutions, for which the point-Universe does not impact against the potential walls. Now we want to verify if the natural evolution of the system, starting from any point in the parameter's space, will bring the point-Universe to the *Kasner stability region*. The calculus of the equation of motion is very complicated because of the potential term, so we will not integrate numerically the equation of motion (which are not clearly analytical integrable) to determinate the evolution of the cosmological model. Instead, recalling the method used by Misner in [34] to find the equation (31) we will search for three constants of motion that allow us to find the new Kasner solution, after the bounce, as a function of the previous solution.

The *superHamiltonian* constraint takes the form:

$$\mathcal{H}_{\rm IX,JF} = \phi\pi_\phi^2 - 2\pi_\phi p_\alpha + \frac{p_+^2+p_-^2}{\phi} + \phi V(\alpha,\beta_\pm) = 0, \tag{59}$$

where the potential of the model is given by equation (56) and the potential $V(\phi)$ was neglected, as we saw previously.

We will solve the *superHamiltonian* constraint with respect to the variable ϕ:

$$\pi_\phi = \frac{1}{\phi}\left\{p_\alpha + \sqrt{p_\alpha^2 - p_+^2 - p_-^2 - \phi^2 V(\alpha,\beta_\pm)}\right\}. \tag{60}$$

In the standard case, the evolution of the Universe is described by giving $\beta_\pm$ as functions of the scalar field ϕ. The entire problem is governed by the function $V(\alpha, \beta_\pm)$, which has the symmetry of an equilateral triangle.

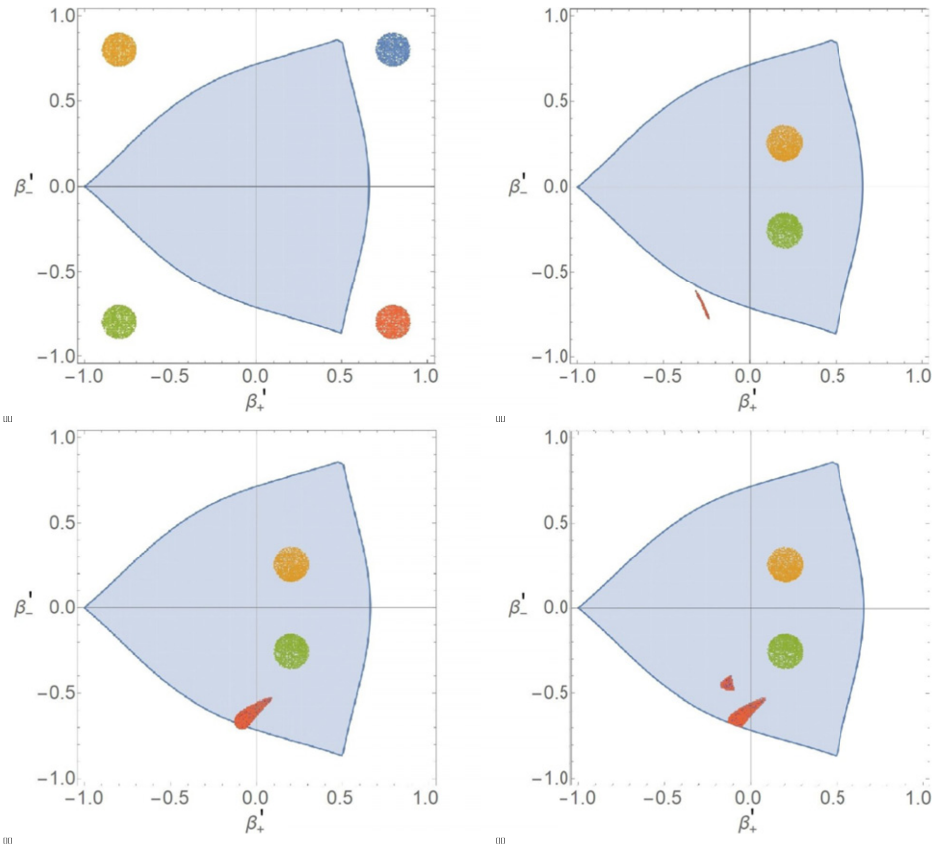

Figure 1. The *Kasner stability region* is the blue region in the plane β'_+, β'_-. In figure is shown the evolution of 10^4 models with different initial conditions. The models are divided in four circles placed at the corners of the square $\beta'_+ < 1$ and $\beta'_- < 1$. The models were evolved thanks to the *Kasner map* (68) which allow us to find the new Kasner solution after the bounce of the point-Universe against the potential wall of the Bianchi IX potential. After three bounce all the models reach the stability region and then no other bounces occur. Thanks to the *Kasner stability region* and *Kasner map* the chaotic behavior of the Bianchi IX model is removed in the context of $f(R)$-gravity in the Jordan frame, in the limit of a negligible potential term of the additional scalar field.

For $\beta_+ \to -\infty$ it gets the following asymptotic form

$$V \sim e^{2\alpha - 4\beta_+}, \tag{61}$$

showing one of the three exponentially steep walls on which the equipotentials are straight lines. The corners of this triangular potential are open, it satisfies the condition $V \geqslant 0$ and vanishes only at the origin, where $V \approx 2\left(\beta_+^2 + \beta_-^2\right)$. Because the potential rises so steeply for large β, little time is spent with the β bouncing against the potential wall and most of the time is spent in free motion when V can be neglected, so the motion is described by the Kasner solutions (41) and (42).

By defining the velocities as the derivatives with respect to the logarithm of scalar field

$$\alpha' = 1 + \frac{p_\alpha}{\sqrt{p_\alpha^2 - p_+^2 - p_-^2}},$$
$$v_\pm = \frac{p_\pm}{\sqrt{p_\alpha^2 - p_+^2 - p_-^2}}, \tag{62}$$

with the condition $(\alpha' - 1)^2 - (\beta'_+)^2 - (\beta'_-)^2 = 1$.

For the sake of simplicity we study the bouncing against the potential of an assigned Kasner solution, considering the vertical wall which intersects the axes β_+. We recall that the choice of this wall is equivalent to any other one, due to the triangular symmetry of the potential (under a rotation of $\frac{\pi}{3}$). We consider the asymptotic form of the *superHamiltonian* using equation (61):

$$\mathcal{H}_{\text{IX,JF}} = \frac{1}{\phi}\left\{p_\alpha + \sqrt{p_\alpha^2 - p_+^2 - p_-^2 - \phi^2\,\mathrm{e}^{+2\alpha-4\beta_+}}\right\}. \tag{63}$$

It is independent of β_- in this approximation, so p_- will be constant during the bounce. Another constant of motion can be found by comparing this equation

$$p'_+ = -\frac{\partial\mathcal{H}_{\text{IX,JF}}}{\partial\beta_+} = 4\mathcal{H}^{-1}_{\text{IX,JF}}\,\mathrm{e}^{2\alpha-4\beta_+},$$
$$p'_\alpha = -\frac{\partial\mathcal{H}_{\text{IX,JF}}}{\partial\alpha} = -2\mathcal{H}^{-1}_{\text{IX,JF}}\,\mathrm{e}^{2\alpha-4\beta_+}, \tag{64}$$

with the results that $\frac{1}{2}p_+ + p_\alpha = \text{const}$. A third constant of motion can be found in the same way, by comparing the two terms

$$\frac{\partial\phi\pi_\phi}{\partial\phi}; \qquad \frac{\partial p_\alpha}{\partial\phi} \tag{65}$$

and so we have $\phi\pi_\phi + p_\alpha = \text{const}$.

Thus, the explicit form of the constants of motion is:

$$\begin{cases} K_1 = 2p_\alpha + \sqrt{p_\alpha^2 - p_+^2 - p_-^2}, \\ K_2 = \dfrac{1}{2}p_+ + p_\alpha, \\ K_3 = p_-. \end{cases} \tag{66}$$

The system of equation we want to solve is: $K_i(p'_\alpha, p'_+, p'_-) = K_i(p_\alpha, p_+, p_-)$, with $i = 1, 2, 3$ and the primate quantities are the ones after the bounce. We chose these three constants of motion to reproduce the analysis of the Mixmaster Universe made by C Misner in GR and properly extend it to $f(R)$ gravity in the Jordan frame.

However, we have to stress that this choice of integrals of the motion is not strictly unique, as typically occurs in general in analytical mechanics: given a set of constant of motions, generic functions of them are still constants of motion for that system. Unless some constant of motion have a clear physical meaning (energy, angular momentum, etc…), the best choice is the simplest one, which makes immediate the dynamics description. We followed here just this criterion to select our constant of motion, having in mind that the physical properties of the Bianchi IX dynamics, like non-integrability and chaoticity, are not affected by the specific form given to the available set.

In order to solve the system we use the Kasner solution to write the equations as function of $v_\pm$ and v_α, with $v_\alpha = \alpha' - 1$. The velocities satisfy the condition: $v_\alpha^2 - v_+^2 - v_-^2 = 1$, which suggest the following change of variables:

$$v_\alpha = \cosh\,\varphi, \qquad v_+ = \sinh\,\varphi\,\cos\,\theta, \qquad v_- = \sinh\,\varphi\,\sin\,\theta. \tag{67}$$

We can rewrite the constant of motion as function of φ and θ:

$$\begin{cases} \tilde{H}(2\,\cosh\,\varphi + 1), \\ \tilde{H}\left(\dfrac{1}{2}\sinh\,\varphi\,\cos\,\theta + \cosh\,\varphi\right), \\ \tilde{H}(\sinh\,\varphi\,\sin\,\theta), \end{cases} \tag{68}$$

where $\tilde{H} = \sqrt{p_\alpha^2 - p_+^2 - p_-^2}$.

We have developed a software to help us to simulate the evolution of the system. We have performed many simulations to understand if the system was able to reach the stability region starting from any point in the space of the parameter that describes the Kasner solutions (β'_+, β'_-). Since $|\beta'_\pm| < 1$ we choose to evolve 10 000 models inside four circles on the four corners of the square with a radius 0.1.

The constants of motion are written as function of v_+ and v_+ while the *Kasner stability region* is a function of $\beta'_\pm$, we can write $\beta'_\pm = \frac{v_\pm}{v_\alpha + 1}$ and evaluate the position of the model in the Kasner parameters' space after every bounce against the potential walls. Every run of the model, started with random parameters inside the circles, has reached the stability region and so we can deduce that the natural evolution of a Bianchi IX cosmology in the Jordan frame naturally removes chaos.

5. Quantum *f*(*R*) cosmology

With the term quantum cosmology (QC) we refer to the application of the quantum theory of gravity to the entire Universe. The existence of such a theory would clarify the physics of the Big Bang, describing the entire Universe like a relativistic-quantum object.

5.1. Bianchi I Universe

By promoting the *superHamiltonian* constraint (32) to a quantum operator annihilating the wave function $\varphi(\alpha, \beta_\pm, \phi)$, we obtain the WDW equation

$$\begin{aligned} \hat{\mathcal{H}}_{\mathrm{B\,I,JF}}|\varphi\rangle &= \frac{2\,\mathrm{e}^{-\frac{3}{2}\alpha}}{\mathbf{v}}\left[\frac{1}{6\phi}\left(\hat{p}_+^2 + \hat{p}_-^2\right) + \frac{1}{6}\hat{\pi}_\phi^2\phi - \frac{1}{3}\hat{p}_\alpha\hat{\pi}_\phi\right]|\varphi\rangle \\ &= \frac{2\,\mathrm{e}^{-\frac{3}{2}\alpha}}{\mathbf{v}}\hbar^2\left[-\frac{1}{6\phi}\left(\partial_+^2 + \partial_-^2\right) - \frac{\phi}{6}\partial_\phi^2 + \frac{1}{3}\partial_\alpha\partial_\phi\right]\varphi = 0. \end{aligned} \tag{69}$$

In the kinetic term mixed impulses in the variables (α, ϕ) appear and consequently, it is impossible to trace the formalism back to the problem of a free relativistic particle. We choose a particular factor ordering of the WDW equation rewriting the equation as

$$\frac{2\,\mathrm{e}^{-\frac{3}{2}\alpha}}{\mathbf{v}}\hbar^2\left[\frac{1}{3}\partial_\alpha\partial_\phi-\frac{1}{6\phi}\left(\partial_+^2+\partial_-^2\right)-\frac{1}{6}\partial_\phi\left(\phi\partial_\phi\right)\right]\varphi=0. \tag{70}$$

Substituting in equation (70) the natural solution

$$\varphi(\alpha,\beta_\pm,\phi)=A\,\mathrm{e}^{\mathrm{i}\left(k_+\beta_++k_-\beta_-+k_\alpha\alpha\right)}f(\phi), \tag{71}$$

we obtain a Bessel differential equation for the function $f(\phi)$

$$\phi^2\frac{\partial^2 f}{\partial\phi^2}+\phi\frac{\partial f}{\partial\phi}(1-2\mathrm{i}k_\alpha)-\left(k_+^2+k_-^2\right)f=0, \tag{72}$$

of solution

$$f(\phi)=c_1\phi^{\mathrm{i}\left(k_\alpha-\sqrt{k_\alpha^2-k_+^2-k_-^2}\right)}\left(c_2+\phi^{2\mathrm{i}\sqrt{k_\alpha^2-k_+^2-k_-^2}}\right), \tag{73}$$

where (c_1, c_2) are arbitrary constants to be fixed by the initial conditions. As is usually done in QC in the presence of a scalar field, we will assume ϕ as a timelike variable. Such a choice, in the Jordan frame is interesting for the idea of using a gravitational degree of freedom as a quantum time. In this way, the problem of time in quantum gravity could be addressed through a generalization of GR. It is worth stressing that the scalar field emerging in the Jordan frame is not physically different from a minimally coupled matter scalar field, apart from the non-trivial coupling with the metric tensor. In [30] it has been shown that this additional degree of freedom is a real massive mode, whose presence introduces new polarizations in the gravitational wave of a $f(R)$ theory, viewed in the Jordan frame. Near the cosmological singularity, we consider as negligible the scalar potential, so that we deal with a free massless non-minimally coupled scalar field, which can play the role of a relational matter clock, in the same way the kinetic term of a self-interacting scalar matter field is commonly adopted in QC to describe the system evolution [41]. Also the interaction with the thermal bath with the non-minimally coupled mode is indistinguishable from a matter field, since both these fields have no a direct coupling with the radiation component. By other words, here we propose that in a modified gravity theory of having the $f(R)$ morphology, a natural clock is provided within its gravitational degrees of freedom, since the non-minimally scalar mode manifests itself as a scalar matter field coupled to standard gravity. We would like to stress that, adopting in quantum gravity a physical clock, as we did for our minisuperspace model choosing ϕ implies that the resulting dynamical picture is the only available for the system. In fact, on a quantum level, it is not possible to pass to a description based on a label time, e.g. the synchronous time. Such a mapping is, in fact, possible only if and when the quantum Universe approaches a classical limit. For an example of the discrepancy existing between the description in terms of an internal clocks and a synchronous time, see [42–44]. However, our choice of ϕ as an internal clock should be regarded as a natural one, since, according to the standard quantum gravity literature [45], we identify an internal scalar degree of freedom as the time coordinate after the quantization procedure is performed. Of course other choices would be possible, for instance the volume of the Universe, but the present analysis makes immediate the comparison to standard geometrodynamics when an external scalar field is considered, according to a large number of cosmological analyzes in the quantum regime [3].

We finally observe that, the possibility to neglect, near enough to the cosmological singularity, the presence of the potential term $V(\phi)$, is of crucial relevance in defining its role of time coordinate. In fact, the presence of such a term could induce a non-monotonical behavior of the scalar field (for instance due to oscillations around the minimum of the potential) and this (in principle classical) feature of the time variable is one of the ground level requirement to deal with a suitable relational clock [46].

One can easily note that, by choosing the variable ϕ as the internal time of the theory, the frequency separation procedure is unfeasible due to the lack of the term $e^{ik_\phi \phi}$. Since the WDW equation (70) is linear, the superposition principle holds, so we can construct the following Gaussian wave packet describing the quantum dynamics of the Bianchi I Universe

$$\Phi(\alpha, \beta_\pm, \phi) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \mathrm{d}k_\alpha\, \mathrm{d}k_+\, \mathrm{d}k_-\, A(k_\alpha, k_\pm)\varphi(\alpha, \beta_\pm, \phi), \tag{74}$$

where we choose

$$A(k_\alpha, k_\pm) = \frac{1}{\sqrt{(2\pi)^3}\sigma_\alpha\sigma_+\sigma_-} \mathrm{e}^{-\left(\frac{(k_\alpha - \bar{k}_\alpha)^2}{2\sigma_\alpha^2} + \frac{(k_+ - \bar{k}_+)^2}{2\sigma_+^2} + \frac{(k_- - \bar{k}_-)^2}{2\sigma_-^2}\right)}, \tag{75}$$

as a Gaussian probability distribution, in order to properly localize the quantum state.

We note that by constructing Gaussian-like wave packets, we are assigning a specific state morphology to our dynamical system, a degree of freedom always ensured by a Cauchy problem for the quantum evolution. The Gaussian states have the peculiarity that their morphology is summarized by the mean value and the standard deviation of the considered configurational coordinate. If we would have considered more generic localized states, the role of the higher probability distribution moments can no longer be disregarded, in principle. Nonetheless, the physical intuition on the spreading properties of the quantum evolution is certainly contained in the Gaussian packets, since their Fourier representation provides an immediate elucidation of the uncertainty relation.

5.1.1. The probability density. In order to define a Hilbert space, we must introduce a positive-defined scalar product and, therefore, a positive-defined probability that is preserved over time. We can build the scalar product induced by the WDW equation (70) by imposing the relation

$$\varphi^*(71) - \varphi(71)^* = 0, \tag{76}$$

where φ^* is the complex conjugate wave function and $(71)^*$ represents the complex conjugate WDW equation. In particular, the relation (76) explicitates as

$$\frac{1}{6\phi}\left(\varphi^*\partial_+^2\varphi - \varphi\partial_+^2\varphi^* + \varphi^*\partial_-^2\varphi - \varphi\partial_-^2\varphi^*\right) + \frac{1}{6}\left(\varphi^*\partial_\phi\left(\phi\partial_\phi\varphi\right) - \varphi\partial_\phi\left(\phi\partial_\phi\varphi^*\right)\right) + \\ - \frac{1}{3}\left(\varphi^*\partial_\alpha\partial_\phi\varphi - \varphi\partial_\alpha\partial_\phi\varphi^*\right) = 0. \tag{77}$$

In order to search for a probability density, we want to trace back the quantity (77) to a continuity equation

$$\partial_\mu J^\mu = 0\ \mu = \left(\alpha, \beta_+, \beta_-, \phi\right). \tag{78}$$

We emphasize that we have relaxed the request to use a covariant four-divergence, in favor of a Minkowskian one. Considering the so-called *minisupermetric* $g^{\mu\nu}$ in the equation (70)

$$g^{\mu\nu} = \begin{pmatrix} 0 & 0 & 0 & -\frac{1}{6} \\ 0 & \frac{1}{6\phi} & 0 & 0 \\ 0 & 0 & \frac{1}{6\phi} & 0 \\ -\frac{1}{6} & 0 & 0 & \frac{\phi}{6} \end{pmatrix} \tag{79}$$

we can explicitate the relation (78) as

$$\partial_\mu J^\mu == \frac{1}{6\phi}\left(\partial_+ J_+ + \partial_- J_-\right) + \frac{1}{6}J_\phi + \frac{\phi}{6}\partial_\phi J_\phi - \frac{1}{6}\partial_\alpha J_\phi - \frac{1}{6}\partial_\phi J_\alpha. \tag{80}$$

By comparing equations (77) and (80), the components of the conserved four-current J^μ take the form

$$\begin{cases} J_\pm = \left(\varphi^*\partial_\pm\varphi - \varphi\partial_\pm\varphi^*\right), \\ J_\phi = \left(\varphi^*\partial_\phi\varphi - \varphi\partial_\phi\varphi^*\right), \\ J_\alpha = \left(\varphi^*\partial_\alpha\varphi - \varphi\partial_\alpha\varphi^*\right), \end{cases} \tag{81}$$

and, in analogy with the KG theory, the quantity

$$\int_{V_\infty} \mathrm{i}J_\phi \, \mathrm{d}\beta_\pm d\alpha = \langle\varphi|\varphi\rangle, \tag{82}$$

turns out to be a good candidate for a probability. However, this scalar product is not positive-defined and, unlike the case of the KG theory, the separation of frequencies cannot be performed. We now define the probability density

$$\rho_\phi = \mathrm{i}\left(\varphi^*\partial_\phi\varphi - \varphi\partial_\phi\varphi^*\right) = \mathrm{i}\left(f^*\partial_\phi f - f\partial_\phi f^*\right). \tag{83}$$

Considering the function f in equation (73)

$$\begin{aligned} f(\phi) &= \phi^{i\left(k_\alpha - \sqrt{k_\alpha^2 - k_+^2 - k_-^2}\right)}\left(1 + \phi^{2i\sqrt{k_\alpha^2 - k_+^2 - k_-^2}}\right) \\ &= \phi^{\mathrm{i}k_\alpha}\left(\phi^{-i\sqrt{k_\alpha^2 - k_+^2 - k_-^2}} + \phi^{i\sqrt{k_\alpha^2 - k_+^2 - k_-^2}}\right), \end{aligned} \tag{84}$$

with the choice $c_1 = c_2 = 1$, the probability density takes the form

$$\rho_\phi = -\frac{2k_\alpha}{\phi}\left(2 + \phi^{-2iR} + \phi^{2iR}\right), \tag{85}$$

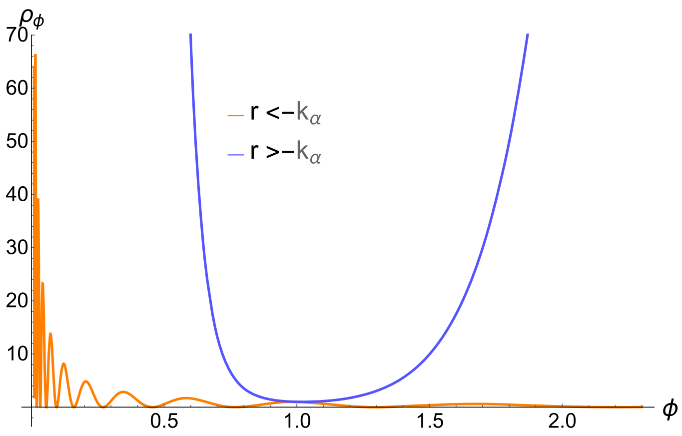

Figure 2. The trend of the probability density ρ_ϕ as a function of the time ϕ. The oscillatory $\cos^2[\ln(\phi)]$ regime is shown in orange; the hyperbolic $\cosh^2[\ln(\phi)]$ regime is shown in blue.

where $R = \sqrt{k_\alpha^2 - k_+^2 - k_-^2}$. Doing some math, we arrange the term in parentheses

$$\begin{aligned}\left(2 + \phi^{-2iR} + \phi^{2iR}\right) &= 2 + \mathrm{e}^{\ln\left(\phi^{2iR}\right)} + \mathrm{e}^{\ln\left(\phi^{-2iR}\right)} \\ &= 2 + \left(\mathrm{e}^{i2R\ \ln(\phi)} + \mathrm{e}^{-i2R\ \ln(\phi)}\right) \\ &= 2 + 2\ \cos(2R\ \ln(\phi)) \\ &= 2[1 + \cos(2R\ \ln(\phi))] = 2\left[2\cos^2\left(\frac{2R\ \ln(\phi)}{2}\right)\right]. \end{aligned} \quad (86)$$

Finally, we can rewrite the probability density (85) as

$$\rho_\phi = -\frac{8k_\alpha}{\phi}\cos^2\left(\ln(\phi)\sqrt{k_\alpha^2 - k_+^2 - k_-^2}\right). \quad (87)$$

It is easy to see that $\rho_\phi \in \mathbb{R}$ and imposing the condition $\rho_\phi > 0$, we find the constraint $k_\alpha < 0$. Using polar coordinates

$$\begin{cases} k_+ = r\ \sin\ \theta, \\ k_- = r\ \cos\ \theta. \end{cases} \quad (88)$$

we can find two trends for the probability density function, depending on whether the term $\sqrt{k_\alpha^2 - k_+^2 - k_-^2} = \sqrt{k_\alpha^2 - r^2}$ is real or imaginary (see figure 2).

In particular, being $r > 0$ and $k_\alpha < 0$,

$$\begin{cases} \text{if } r < -k_\alpha & \text{oscillatory } \cos^2[\ln(\phi)]\text{regime}, \\ \text{if } r > -k_\alpha & \text{hyperbolic } \cosh h^2[\ln(\phi)]\text{regime}. \end{cases} \quad (89)$$

Considering the condition (40) derived from the Hamilton's equations and the relation $p = \hbar k$, we conclude that only the oscillatory regime is physically acceptable. Therefore, the wave packet (74) can be rewritten as

$$\Phi(\alpha,\beta_\pm,\phi)=\int_{-\infty}^{0}\int_{0}^{-k_\alpha}\int_{0}^{2\pi}\mathrm{d}k_\alpha\,\mathrm{d}r\,\mathrm{d}\theta\;[rA(k_\alpha,r,\theta)\varphi(\alpha,\beta_\pm,\phi)], \tag{90}$$

where

$$A(k_\alpha,r,\theta)=\frac{1}{\sqrt{(2\pi)^3}\sigma_\alpha\sigma_+\sigma_-}\mathrm{e}^{-\left(\frac{(k_\alpha-\bar{k}_\alpha)^2}{2\sigma_\alpha^2}+\frac{(r\,\sin\,\theta-\overline{r\,\sin\,\theta})^2}{2\sigma_+^2}+\frac{(r\,\cos\,\theta-\overline{r\,\cos\,\theta})^2}{2\sigma_-^2}\right)}. \tag{91}$$

Consequently, the normalizable probability density is

$$\rho_\phi=\mathrm{i}\left(\Phi^*\partial_\phi\Phi-\Phi\partial_\phi\Phi^*\right). \tag{92}$$

5.2. The isotropic and homogeneous FLRW Universe

In this section, we will analyze the quantum behavior of the FLRW Universe in the context of the $f(R)$-gravity in the Jordan frame. In the assumption $\beta_\pm=0$ (and hence $p_\pm=0$) the *superHamiltonian* (32) reduces to the simpler form

$$\mathcal{H}_{\text{FLRW,JF}}=\frac{2\,\mathrm{e}^{-\frac{3}{2}\alpha}}{\mathbf{v}}\left[\frac{1}{6}\pi_\phi^2\phi-\frac{1}{3}p_\alpha\pi_\phi\right], \tag{93}$$

and quantum dynamics is described by the WDW equation

$$\frac{2\,\mathrm{e}^{-\frac{3}{2}\alpha}}{\mathbf{v}}\hbar^2\left[-\frac{1}{6}\partial_\phi\left(\phi\partial_\phi\right)+\frac{1}{3}\partial_\alpha\partial_\phi\right]\varphi(\alpha,\phi)=0. \tag{94}$$

We note that the quantization of a homogeneous and isotropic model has no clear physical meaning, since we lost the two Einstenian gravitation degrees of freedom. In this respect, we can infer that the quantization of the FLRW Universe must be mainly regarded as a toy model on which the different QC approaches can be easily tested. Considering the natural solution

$$\varphi=A\,\mathrm{e}^{\mathrm{i}k_\alpha\alpha}f(\phi), \tag{95}$$

we obtain a second-order differential equation for the function $f(\phi)$

$$\phi\frac{\partial^2 f}{\partial\phi^2}+\frac{\partial f}{\partial\phi}(1-2\mathrm{i}k_\alpha)=0, \tag{96}$$

having as solution

$$f(\phi)=c_1+c_2\left(\frac{1}{2\mathrm{i}k_\alpha}\right)\phi^{2\mathrm{i}k_\alpha}. \tag{97}$$

5.2.1. Time before quantization: the ADM reduction method. In the model under examination, we consider the variable ϕ as the embedding variable and the Misner variable α as the physical degree of freedom. Solving classically the *superHamiltonian* constraint with respect to the conjugate momentum π_ϕ we derive the equation

$$\pi_\phi\left(\frac{1}{6}\pi_\phi\phi-\frac{1}{3}p_\alpha\right)=0, \tag{98}$$

having as solutions

$$\begin{cases} \pi_{\phi,1} = 0, \\ \pi_{\phi,2} = \dfrac{2p_\alpha}{\phi}. \end{cases} \tag{99}$$

Considering the non-trivial one, we can define

$$h_\phi = -\frac{2p_\alpha}{\phi}, \tag{100}$$

as the physical Hamiltonian that regulates the dynamics with respect to the time ϕ. The next step consists in the imposition of the so-called time gauge

$$\dot{\phi} = N\frac{\partial \mathcal{H}_{\mathrm{FLRW,JF}}}{\partial \pi_\phi} = \frac{2N\,\mathrm{e}^{-\frac{3}{2}\alpha}}{\mathbf{v}}\left(\frac{1}{3}\pi_\phi\phi - \frac{1}{3}p_\alpha\right) = 1, \tag{101}$$

which sets the lapse function N

$$N = N_{\mathrm{ADM}} = \frac{3\mathbf{v}\,\mathrm{e}^{\frac{3}{2}\alpha}}{2\left(\pi_\phi\phi - p_\alpha\right)}, \tag{102}$$

and allows us to write the reduced action

$$S_{\mathrm{red}} = \int \mathrm{d}\phi\left(p_\alpha\frac{\partial\alpha}{\partial\phi} - h_\phi\right). \tag{103}$$

The Hamilton's equations are defined as

$$\begin{cases} \dfrac{\partial\alpha}{\partial\phi} = \dfrac{\partial h_\phi}{\partial p_\alpha} = -\dfrac{2}{\phi}, \\ \dfrac{\partial p_\alpha}{\partial\phi} = -\dfrac{\partial h_\phi}{\partial\alpha} = 0, \end{cases} \tag{104}$$

from which we obtain the classical trajectory with respect to time ϕ

$$\alpha(\phi) = -2\,\ln(\phi) + \alpha_0 = -2\,\ln(\phi), \tag{105}$$

where we have set $\alpha_0 = \alpha(0) = 0$.

5.3. The probability density and the comparison between the classical trajectory and quantum evolution

In analogy to the case of the Bianchi I Universe we want to define a Hilbert space through the introduction of the probability density

$$\rho_\phi = \mathrm{i}\left(\varphi^*\partial_\phi\varphi - \varphi\partial_\phi\varphi^*\right). \tag{106}$$

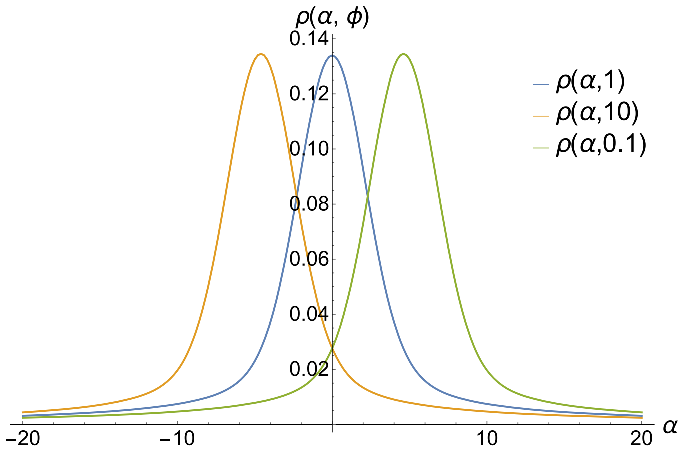

Figure 3. The trend of the probability density $\rho(\alpha, \phi)$ as a function of the coordinate α for different values of ϕ. $\phi = 0.1$ is shown in green; $\phi = 1$ is shown in blue; $\phi = 10$ is shown in orange.

Replacing the wave function (95) assuming $c_1 = 0, c_2 = 1$, we obtain the non-normalized probability density

$$\rho_\phi = -\frac{1}{k_\alpha \phi}, \tag{107}$$

which is positive if $k_\alpha < 0$. Considering that there are no monochromatic physical wave functions, we construct the Gaussian wave packet which is a solution of the WDW equation (94)

$$\Phi(\alpha, \phi) = \int_{-\infty}^{0} \mathrm{d}k_\alpha A(k_\alpha) \mathrm{e}^{\mathrm{i}k_\alpha \alpha} \left(\frac{1}{2\mathrm{i}k_\alpha}\right) \phi^{2\mathrm{i}k_\alpha}, \tag{108}$$

where

$$A(k_\alpha) = \frac{1}{\sqrt{(2\pi)}\sigma_\alpha} \mathrm{e}^{-\left(\frac{(k_\alpha - \bar{k}_\alpha)^2}{2\sigma_\alpha^2}\right)}. \tag{109}$$

The normalized probability density

$$\rho_\phi = \mathrm{i}\left(\Phi^* \partial_\phi \Phi - \Phi \partial_\phi \Phi^*\right), \tag{110}$$

gives the probability of finding the FLRW Universe at a certain instant ϕ per unit of 'spatial coordinate' α.

We now study the trend of the quantity (110) with respect to $\phi > 0$ as we can see from (105) (see figure 3).

From figure 3 we see that there's no spreading of the wave packet and the probability density remains perfectly localized over time. We now prove the validity of the Ehrenfest theorem by comparing the classical trajectory provided by Hamilton's equations and the values of the coordinates α corresponding to the maximums of the probability density ρ_ϕ as ϕ varies (strictly speaking, we should study the expectation value $\langle \Phi | \hat{\alpha} | \Phi \rangle$, but for highly localized

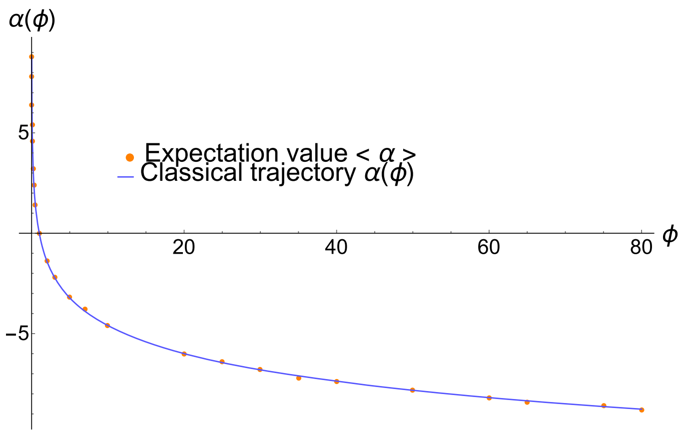

Figure 4. Comparison between the classical trajectory (solid blue line) and the values $\alpha(\phi)$ where the probability density is maximally localized as ϕ varies (dotted orange line).

Gaussian probability density the values of α where there's a maximum is a good approximation). From figure 4 it is evident that the quantum dynamics perfectly follows the classical dynamics of the FLRW Universe in the Jordan frame. This result demonstrates that such a quantum-cosmological model reaches the singularity ($\phi \to +\infty$) in a classical way, allowing us to consider the quantum effects in the Planckian regime, as effects of lower order on a semiclassical Universe. It should be emphasised that the proposed quantization is not capable of solving the problem of the presence of the classical singularity and, therefore, is not a satisfactory solution to this still open problem.

5.4. Comparison with the FLRW model filled with a scalar field in general relativity

The WDW equation in Misner variables for the FLRW Universe in GR filled with a minimally coupled scalar field ϕ is

$$\begin{aligned}\mathcal{H}_{\mathrm{FLRW}+\phi} &= \frac{2\,\mathrm{e}^{-\frac{3}{2}\alpha}}{\mathbf{v}}\left[-\hat{p}_\alpha^2 + \hat{\pi}_\phi^2\right]|\varphi\rangle \\ &= \frac{2\,\mathrm{e}^{-\frac{3}{2}\alpha}}{\mathbf{v}}\left(\partial_\alpha^2 - \partial_\phi^2\right)\varphi(\alpha,\phi) = 0,\end{aligned} \tag{111}$$

where we neglected the potential term $U(\phi)$ related to the derivatives of the scalar field. Differently from the case (94) in the Jordan frame, this equation resembles a two-dimensional KG equation describing a free and massless particle, where the external scalar field ϕ plays the role of the time variable. The wave function φ solution of the equation is a plane wave

$$\varphi(\alpha,\phi) = A\,\mathrm{e}^{\mathrm{i}\left(k_\alpha \alpha + k_\phi \phi\right)}, \tag{112}$$

and assuming a Gaussian wave packet at the initial time ϕ_0, we write the general solution

$$\Phi(\alpha,\phi) = \int_{-\infty}^{0} \mathrm{d}k\, A(k)\mathrm{e}^{\mathrm{i}k(\alpha+\phi)}, \tag{113}$$

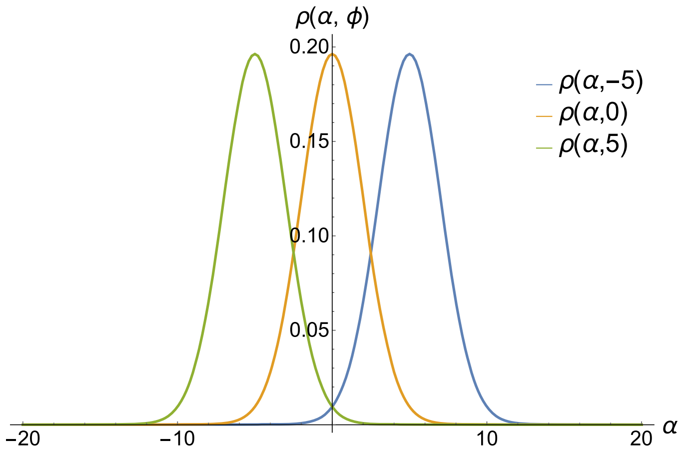

Figure 5. Evolution of the probability density $\rho(\alpha, \phi)$ as a function of the coordinate α for different values of ϕ. $\phi = 0$ is shown in orange; $\phi = 5$ is shown in green; $\phi = -5$ is shown in blue.

where

$$A(k) = \frac{1}{\sqrt{(2\pi)}\sigma}\mathrm{e}^{-\left(\frac{\left(k-\bar{k}\right)^2}{2\sigma^2}\right)}, \tag{114}$$

and $k \equiv k_\phi = k_\alpha < 0$. Through the study of the probability density

$$\rho_\phi = \mathrm{i}\left(\Phi^*\partial_\phi\Phi - \Phi\partial_\phi\Phi^*\right), \tag{115}$$

we can infer the absence of the spreading phenomenon typical of a free quantum particle (figure 5).

We conclude that even in the case of GR with a minimally coupled scalar field, the FLRW Universe admits a classical limit valid up to Planckian regimes. In support of this claim, we apply the ADM reduction procedure and derive the Hamilton's equations

$$\begin{cases} \dfrac{\partial\alpha}{\partial\phi} = \dfrac{\partial h_\phi}{\partial p_\alpha} = -\dfrac{1}{2\sqrt{p_\alpha}} \\ \dfrac{\partial p_\alpha}{\partial\phi} = -\dfrac{\partial h_\phi}{\partial\alpha} = 0 \end{cases} \tag{116}$$

from which the classical trajectory takes the form

$$\alpha(\phi) = -c\phi \tag{117}$$

where c is a constant of the motion.

From figure 6 it emerges that quantum dynamics perfectly follows the classical dynamics of the FLRW Universe filled with a minimally coupled scalar field. Furthermore, it is possible to fix the constant of motion $c = 1$. In conclusion, we stress two main differences between the two models under consideration: the first one is the linear vs logarithmic trend of $\alpha(\phi)$ with

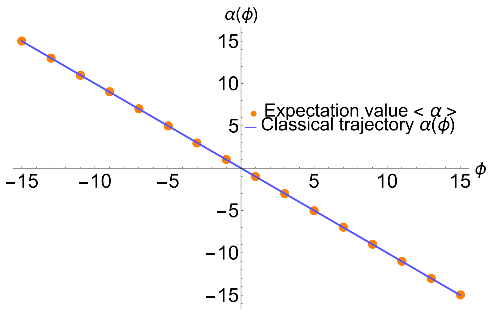

Figure 6. Comparison between the classical trajectory (solid blue line) and the values $\alpha(\phi)$ where the probability density is maximally localized as ϕ varies (dotted orange line).

which the singularity is approached; the second one is the range of values assumed by the time variable ϕ which, in the case of the Jordan frame, was limited only to the positive semi-axis of the real numbers. In both models, however, the canonical quantization based on the WDW formalism does not solve the problem of the existence of a cosmological singularity, paving the way for different theoretical approaches.

6. Concluding remarks

In this paper, we provided a systematic and detailed analysis of the cosmological implication of an $f(R)$-gravity in the Jordan frame, especially in the limit of a negligible potential term of the non-minimally coupled scalar field. Some interesting results have been clearly stated and here briefly re-analyzed. As first step, we show in the general Hamiltonian formulation, as well as in its implementation to the dynamics of a generic Universe, that if we use the three-metric determinant as a separated variable, like in [22], its conjugate momentum enters linearly only in the scalar Hamiltonian constraint. Differently from what it takes place in the standard WDW equation, we are here always able to set up a Schrödinger formulation in which the three-determinant plays the role of a time variable, although the associated Hamiltonian turns out to be a non-local functional operator. The second very significant result we developed consists of the proof that the Bianchi IX cosmology is no longer characterized by a chaotic dynamics in an extended $f(R)$ theory of gravity, as soon as the potential term bringing the information on the form of f is negligible near to the singularity. Here we adopted Misner variables to describe the Bianchi IX line element and we demonstrated both the existence and the attractivity of a Kasner stability region. The definition of the region where a Kasner regime becomes stable is derived analytically, while the proof that the system always reaches such a configuration has been performed on a numerical level. This latter study relies on the existence of three constants of the motion and it can be regarded as the natural generalization of the original Misner approach [34]. The result obtained here about the chaos suppression is coherent with the analysis in [18], where the same issue is discussed using a $f(R)$ approach in the so-called Einstein framework and adopting Misner–Chitré-like variables. Finally, we touch the question of the canonical quantization of the Bianchi I dynamics, concentrating our attention to the quantum evolution of a isotropic Universe. For the Bianchi I, the WDW equation is constructed and a conserved current and a probability density are identified by interpreting the non-minimal scalar field as the internal time variable. A localized wave packet is then constructed for the isotropic Universe and we show how the singularity is still present in such a quantum scenario. Furthermore a comparison between the evolutionary cosmologies using as internal time a minimally and a non-minimally coupled scalar field respectively is provided. Apart from a different dynamics of the peak of the localized packet, we clarify how the non-minimally coupled scalar field emerging in a Jordan frame is a valuable internal time and opens a new point of view on the interpretation of modified $f(R)$ theory of gravity: the additional scalar mode, summarizing the functional form f, can be interpreted as a time-like degree of freedom for the gravitational quantum dynamics, although a viable approach could also emerge by dealing as stressed above, with the three-metric determinant. Since the Bianchi model dynamics has paradigmatic features of the generic inhomogeneous cosmology, we are lead to infer that the present analysis has a relevant impact on a more general sector of the cosmological problem. However, it must be recalled that, when the potential term, associated to the non-minimally coupled scalar field is no longer negligible near the singularity, its presence can significantly affect the validity of some of the present issues, including the non-chaoticity of the Bianchi IX Universe.

Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

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References

[1] Turner M and Kolb E 1990 *The Early Universe* (Boca Raton, FL: CRC Press)
[2] Cianfrani F, Lecian O M, Lulli M and Montani G 2014 *Canonical Quantum Gravity: Fundamentals and Recent Developments* (Singapore: World Scientific)
[3] Montani G, Battisti M V, Benini R and Imponente G 2011 *Primordial Cosmology* (Singapore: World Scientific)
[4] Thorne K S, Misner C W and Wheeler J A 2000 *Gravitation* (San Francisco, CA: Freeman)
[5] Joyce A, Jain B, Khoury J and Trodden M 2015 Beyond the cosmological standard model *Phys. Rep.* **568** 1–98
[6] Landau L D and Lifshitz E M 2013 *The Classical Theory of Fields* vol 2 (Amsterdam: Elsevier)
[7] Burd A B, Buric N and Ellis G F R 1990 A numerical analysis of chaotic behaviour in Bianchi IX models *Gen. Relativ. Gravit.* **22** 349–63
[8] Ringström H 2001 The Bianchi IX attractor *Ann. Henri Poincare* **2** 405–500
[9] Hobill D, Burd A and Coley A (NATOSA Division) 1994 *Deterministic Chaos in General Relativity* vol 322 (*NATO ASI Series B*) (New York: Springer) https://books.google.it/books?id=LUgsAAAAYAAJ
[10] Belinskii V A, Khalatnikov I M and Lifshitz E M 1982 A general solution of the Einstein equations with a time singularity *Adv. Phys.* **31** 639–67
[11] Belinskij V A, Khalatnikov I M and Lifshits E M 1970 Oscillatory approach to a singular point in the relativistic cosmology *Adv. Phys.* **19** 525–73
[12] Sotiriou T P 2015 *Gravity and Scalar Fields* (New York: Springer) pp 3–24
[13] Sotiriou T P and Faraoni V 2010 $f(R)$ theories of gravity *Rev. Mod. Phys.* **82** 451–97

[14] Nojiri S, Odintsov S D and Oikonomou V K 2017 Modified gravity theories on a nutshell: inflation, bounce and late-time evolution *Phys. Rep.* **692** 1–104
[15] Berti E *et al* 2015 Testing general relativity with present and future astrophysical observations *Class. Quantum Grav.* **32** 243001
[16] Bamba K, Capozziello S, Nojiri S. i. and Odintsov S D 2012 Dark energy cosmology: the equivalent description via different theoretical models and cosmography tests *Astrophys. Space Sci.* **342** 155–228
[17] Capozziello S, Carlevaro N, De Laurentis M, Lattanzi M and Montani G 2013 Cosmological implications of a viable non-analytical $f(R)$ model *Eur. Phys. J. Plus* **128** 155
[18] Moriconi R, Montani G and Capozziello S 2014 Chaos removal in $r + qR^2$ gravity: the Mixmaster model *Phys. Rev.* D **90** 101503
[19] Lecian O M and Montani G 2008 Exponential Lagrangian for the gravitational field and the problem of vacuum energy *Int. J. Mod. Phys.* A **23** 1286
[20] Nojiri S and Odintsov S D 2011 Unified cosmic history in modified gravity: from $f(R)$ theory to Lorentz non-invariant models *Phys. Rep.* **505** 59–144
[21] Zhang X and Ma Y 2011 Extension of loop quantum gravity to $f(R)$ theories *Phys. Rev. Lett.* **106** 171301
[22] DeWitt B S 1967 Quantum theory of gravity. I. the canonical theory *Phys. Rev.* **160** 1113–48
[23] Arnowitt R, Deser S and Misner C W 1960 Canonical variables for general relativity *Phys. Rev.* **117** 1595–602
[24] Kirillov A. 1993 On the nature of the spatial distribution of metric inhomogeneities in the general solution of the Einstein equations near a cosmological singularity *Z. Eksp. Teor. Fiz.* **103** 721–9
[25] Imponente G and Montani G 2002 On the quantum origin of the Mixmaster chaos covariance *Nucl. Phys.* B **104** 193–6
[26] Montani G, Battisti M V, Benini R and Imponente G 2008 Classical and quantum features of the Mixmaster singularity *Int. J. Mod. Phys.* A **23** 2353–503
[27] Bahamonde S, Odintsov S D, Oikonomou V K and Wright M 2016 Correspondence of $f(R)$ gravity singularities in Jordan and Einstein frames *Ann. Phys.* **373** 96–114
[28] Deruelle N, Sendouda Y and Youssef A 2009 Various Hamiltonian formulations of $f(\mathcal{R})$ gravity and their canonical relationships *Phys. Rev.* D **80** 084032
[29] Bombacigno F, Boudet S and Montani G 2021 Generalized Ashtekar variables for Palatini $f(R)$ models *Nucl. Phys.* B **963** 115281
[30] Moretti F, Bombacigno F and Montani G 2019 Gauge invariant formulation of metric $f(R)$ gravity for gravitational waves *Phys. Rev.* D **100** 084014
[31] Wilson-Ewing E 2018 The loop quantum cosmology bounce as a Kasner transition *Class. Quantum Grav.* **35** 065005
[32] Antonini S and Montani G 2019 Singularity-free and non-chaotic inhomogeneous Mixmaster in polymer representation for the volume of the universe *Phys. Lett.* B **790** 475–83
[33] Misner C W 1969 Mixmaster universe *Phys. Rev. Lett.* **22** 1071–4
[34] Misner C W 1969 Quantum cosmology. I *Phys. Rev.* **186** 1319–27
[35] Francisco G and Matsas G E A 1988 Qualitative and numerical study of Bianchi IX models *Gen. Relativ. Gravit.* **20** 1047–54
[36] Latifi A, Musette M and Conte R 1994 The Bianchi IX (Mixmaster) cosmological model is not integrable *Phys. Lett.* A **194** 83–92
[37] Boyanovsky D 2015 Effective field theory during inflation: reduced density matrix and its quantum master equation *Phys. Rev.* D **92** 023527
[38] Sharma A K and Verma M M 2022 Power-law inflation in the $f(R)$ gravity *Astrophys. J.* **926** 29
[39] AlHallak M, AlRakik A, Chamoun N and El-Daher M S 2022 Palatini $f(R)$ gravity and variants of k-/constant roll/warm inflation within variation of strong coupling scenario *Universe* **8** 126
[40] Berger B K 1999 Influence of scalar fields on the approach to a cosmological singularity *Phys. Rev.* D **61** 023508
[41] Ashtekar A, Pawlowski T and Singh P 2006 Quantum nature of the Big Bang *Phys. Rev. Lett.* **96** 141301
[42] Bombacigno F, Cianfrani F and Montani G 2016 Big-bounce cosmology in the presence of Immirzi field *Phys. Rev.* D **94** 064021

[43] Montani G, Mantero C, Bombacigno F, Cianfrani F and Barca G 2019 Semiclassical and quantum analysis of the isotropic universe in the polymer paradigm *Phys. Rev.* D **99** 063534
[44] Pawłowski T and Ashtekar A 2012 Positive cosmological constant in loop quantum cosmology *Phys. Rev.* D **85** 064001
[45] Isham C J 1992 Canonical quantum gravity and the problem of time (arXiv:gr-qc/9210011)
[46] Rovelli C 1991 Time in quantum gravity: an hypothesis *Phys. Rev.* D **43** 442–56