

Inflation from non-minimally coupled scalar field in loop quantum cosmology

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The FRW model with non-minimally coupled massive scalar field has been investigated in LQC framework. Considered form of the potential and coupling allows applications to Higgs driven inflation. Out of two frames used in the literature to describe such systems: Jordan and Einstein frame, the latter one is applied. Specifically, we explore the idea of the Einstein frame being the natural 'environment' for quantization and the Jordan picture having an emergent nature. The resulting dynamics qualitatively modifies the standard bounce paradigm in LQC in two ways: (i) the bounce point is no longer marked by critical matter energy density, (ii) the Planck scale physics features the "mexican hat" trajectory with two consecutive bounces and rapid expansion and recollapse between them. Furthermore, for physically viable coupling strength and initial data the subsequent inflation exceeds 60 e-foldings.

I. INTRODUCTION

The inflation paradigm is one of the most successful ideas allowing to explain recent precise cosmological observations. However one of its main problems is the construction of the physically viable scenario featuring sufficiently long inflation epoch (> 60 e-foldings) with sufficiently large probability. In this context a lot of hope is attached to the models featuring a non-minimal coupling of gravity and a scalar field (e.g. the Higgs field [1–3]), vector fields [4] as well as fermions [5] (more precisely, the scalar degrees of freedom generated by the latter). Such mechanism of driving the inflation is also efficient in generating the correct primordial curvature perturbations.

Among the considered scenarios the most popular one corresponds to a coupling of the form $\frac{1}{2}\xi\phi^2R$, where R is the Ricci scalar and ϕ is a scalar field. The non-minimally coupled scalar inflaton drives the slow-roll inflation as long as the non-minimal(ity of the) coupling is strong, i.e. for $\xi\phi^2 \gg 1$. Values of self-coupling constant of scalar field are determined by the normalization of initial inhomogeneities. For example, for the scalar field potential of the form $V(\phi) = \frac{\lambda}{4}(\phi^2 - 2m^2/\lambda)^2$ the agreement with the observations (best fit) sets the self-coupling to $\xi \sim 47000\sqrt{\lambda}$. In this case, the mass term does not have a significant contribution either to the effective potential of the field, or to the normalization of inhomogeneities. Thus, m may be of order of electroweak scale, as in the case of Higgs field or a scalar originating from some extension of the Standard Model. Thus, one is able to explain the whole cosmological data by a minimal amount of new physics. Note that besides some differences pointed out in [6], inflation from a non-minimally coupled scalar field is similar to inflation in $f(R) = R + \epsilon R^2$ gravity [7].

At this point it is worth noting that the type of the potential considered, while usually associated with the models of Higgs inflation, is not restricted just to this particular field. In fact, our studies can be easily (generalized and) applied to the analysis of the inflation driven by any non-minimally coupled scalar field with realistic values of ξ and λ .

The analysis of the running of the coupling constant λ limits the allowed range of m . In case of Higgs field $m \in (126\text{GeV}, 194\text{GeV})$ [8] with the theory error of order of 2GeV . Thus, recent results from CMS [9] and ATLAS [10] ($m_H \simeq 125\text{GeV}$) are both consistent with SM Higgs inflation.

While the considered model is very successful on the classical level it still suffers the standard problems related with the presence of initial singularity, which are expected to be solved by quantum gravity. One of the leading approaches to provide quantum description of spacetime itself is Loop Quantum Gravity (LQG) [11–13]. The cosmological application of its symmetry reduced version, known as Loop Quantum Cosmology (LQC) [14, 15], has indeed provided a qualitatively new picture of early Universe dynamics. The prediction of the so-called *big bounce* phenomenon [16] offered a new mechanism of resolving long standing cosmological problems. For example, the existence of a pre-bounce epoch of the Universe evolution provides an easy solution to the horizon problem, while preliminary studies

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indicate that the dynamics in the near-bounce superinflation epoch prevents the catastrophic entropy increase [17] usually considered a danger to bouncing cosmological models (following the consideration of [18]). What is even more important, the spacetime discreteness effects amount to a dramatic increase of the probability of inflation in the models with standard $m^2\phi^2$ potential scalar fields [19] (see also [20]). Indeed for such models the probability of inflation with enough e -foldings to ensure consistence with 7 years WMAP data happens with probability greater than 0.999997. These results make the loop approach very attractive in inflationary cosmology.

The issue of LQC corrections to models non-minimally coupled to gravity has been analyzed in [21], where the authors have introduced the LQC correction for small values of non-minimal coupling, which were not consistent with observations. The loop quantisation in the context of non-minimal coupling in scalar-tensor theories was considered for example in [22]. In this paper we consider the model of FRW flat universe with scalar field coupled non-minimally to gravity with the realistic values of the constants λ , ξ . In consequence the model features all the regimes of: strong ($|\xi|\phi^2 \gg 1$), medium ($\xi^2\phi^2 > 1, \xi\phi^2 < 1$), and weak ($|\xi|\phi^2 \ll 1$) non-minimal coupling.¹

In the literature the non-minimally coupled scalar field is usually investigated via two approaches: direct calculation in the frame defined by the action (called Jordan frame, see e.g.[23]) and using certain conformal transformation to the frame in which the field is minimally coupled to gravity [24]. It is claimed that these two approaches lead to nonequivalent results [23, 25, 26]. The issue as to which one is the correct candidate for quantization is still open. In this paper we explore (with a slight modification) one of these possibilities, in order to test the viability² of the model resulting from the choice. Namely, we probe the idea, that the observed physics is native to Jordan frame [3], however we take the point of view that it is just an emergent theory, following from the underlying “fundamental” theory described by Einstein frame (see sect. III for more extensive discussion and justification). It is thus the latter one which is subject to the loop quantization in our work.

The structure of this paper is the following: In section II we introduce the model and determine the resulting equations of motion for a scalar field non-minimally coupled to gravity. In section III we perform a canonical transformation (to the so-called Einstein frame), which allows us to recast the theory as the one with minimally coupled matter. In section IV the canonical quantization of Ashtekar-Barbero variables is carried out in the Einstein frame via methods of LQC giving precisely defined quantum framework. This framework is next used in section V as the background for constructing the effective semiclassical description of the system’s dynamics. The resulting semiclassical equations of motion are then applied in section VI in the systematic analysis of the dynamical evolution of the universes described by the model. Its results are presented in section VII. Their general discussion involving in particular the treatment’s limitations is provided in the concluding section VIII.

II. NON-MINIMALLY COUPLED SCALAR FIELD

We start with the general (non-symmetry reduced) system of gravity non-minimally coupled to the massive scalar field, as defined by the following action

$$S[\phi, g_{\mu\nu}] = \frac{1}{8\pi G} \int d^4x \mathcal{L} = \frac{1}{8\pi G} \int d^4x \sqrt{-g} \left[-U(\phi)R + \frac{1}{2}(\partial_\mu\phi)(\partial^\mu\phi) - V(\phi) \right], \quad (2.1)$$

where the chosen metric tensor signature is $(+, -, -, -)$, R is the Ricci scalar and ϕ is a scalar field (which can be the inflaton, Higgs field, modulus field etc). Notice that the limit of minimally coupled scalar field corresponds to $U(\phi) = 1/2$. For the further studies we choose one of the most popular forms of coupling, namely

$$U(\phi) = \frac{1}{2} + \frac{1}{2}\xi\phi^2. \quad (2.2)$$

We will assume that such a non-minimally coupled scalar field ϕ is the dominant matter content in the Universe.

We next reduce the above action to the case of flat FRW spacetime $g = N^2 dt^2 - a^2(t) \delta q^3$. Then, after integration by parts the $Ua^2\ddot{a}$ term, one gets the reduced action

$$S = \frac{1}{8\pi G} \int d^4x a^3 \left[-6UH^2 - 6HU'\dot{\phi} + \frac{1}{2}\dot{\phi}^2 - V \right], \quad (2.3)$$

where $U'(\phi) := [\partial_\phi U](\phi)$.

¹ In this paper values of the inflaton are given in the units of reduced Plack mass $M_{pl} \simeq 2.44 \times 10^{18} GeV$.

² Here as *viable* we consider a model whose predictions do not lead to immediate contradictions with observations.

³ The issue of a scalar field non-minimally coupled to gravity with non-zero spatial curvature was considered e.g. in [27].

By varying this action with respect to a and ϕ , we obtain the following equations of motion:

$$\ddot{\phi} + 3H\dot{\phi} + V' = 6U' \left(\frac{\ddot{a}}{a} + H^2 \right), \quad (2.4a)$$

$$2U'\ddot{\phi} + 2U \left(\frac{2\ddot{a}}{a} + H^2 \right) + 2U''\dot{\phi}^2 + 4HU'\dot{\phi} = -8\pi GP, \quad (2.4b)$$

where $P = \dot{\phi}^2/2 - V$ is the pressure of the scalar field. In the equations above the lapse function has been set to $N = 1$, although at this level it can safely be left unfixed. The variation $\delta S/\delta N = 0$ over it produces the (symmetry-reduced) scalar constraint $\mathbf{H} = 0$, where \mathbf{H} is the Hamiltonian of the scalar field, curvature and their coupling. To define it, let us introduce canonical momenta of the scalar field and of the scale factor:

$$\pi_\phi = \frac{\partial \mathcal{L}}{\partial \dot{\phi}} = a^3 \dot{\phi} - 6U' \dot{a} a^2, \quad \pi_a = \frac{\partial \mathcal{L}}{\partial \dot{a}} = -12U \dot{a} a - 6U' \dot{\phi} a^2. \quad (2.5)$$

For $N = 1$ the Hamiltonian \mathbf{H} takes the form

$$\mathbf{H} = \pi_\phi \dot{\phi} + \pi_a \dot{a} - \mathcal{L} = -6U \dot{a}^2 a - 6U' \dot{\phi} \dot{a} a^2 + a^3 8\pi G \rho, \quad (2.6)$$

where ρ is the energy density of the scalar field. Then the constraint $\mathbf{H} = 0$ implies

$$UH^2 + HU'\dot{\phi} = \frac{8\pi G}{6} \rho. \quad (2.7)$$

Finally, combining the eq. (2.4a-2.7) one obtains the 2nd order equation of motion for ϕ in which the curvature is felt only through the cosmic friction term

$$\ddot{\phi} + 3H\dot{\phi} = \frac{2U'V - UV' - U'\dot{\phi}^2(3U'' + \frac{1}{2})}{U + 3U'^2}, \quad (2.8)$$

where, as before “ $\dot{}$ ” denotes the derivative over ϕ .

Inflation from strong value of non-minimal coupling

Let us introduce the slow-roll parameters defined as follows

$$\epsilon = -\frac{\dot{H}}{H^2}, \quad \eta = \frac{\ddot{H}}{\dot{H}H}. \quad (2.9)$$

The universe is considered to be in the slow-roll inflation epoch whenever $\epsilon, |\eta| \ll 1$ for an extended time. For the coupling as in (2.2) and the potential $V(\phi) = \frac{\lambda}{4}\phi^4$ these parameters can be estimated in the range of strong non-minimal coupling to be

$$\epsilon \propto \eta \propto \frac{1}{\xi \phi^2}. \quad (2.10)$$

It follows then that one obtains slow-roll evolution whenever $\xi \phi^2 > 1$, so inflation ends only when the field leaves the strong coupling regime.

It is worth noting, that (in the considered scenario) during the inflation, $\phi \sim O(\xi^{-1/2}) \ll M_{pl}$. This implies, that there is no need to consider non-renormalizable terms in the potential, as here they shall be suppressed by the Planck scale. This is a theoretical advantage of Higgs inflation over chaotic inflation models (in which $\phi > M_{pl}$ during inflation). Also, despite the Standard Model Higgs field being a complex one, the phase of a field may be expressed by a massless scalar degree of freedom (which does not have a significant influence on the evolution of space-time). It follows then that there is no qualitative difference between the dynamics of our simple model and of a more realistic Higgs-driven inflation. For details, see [27]. In consequence, our considerations can be applied to the physically relevant case

III. TRANSFORMATION TO EINSTEIN FRAME

An alternative approach to describing the system defined in the previous section is its transformation to the so-called ‘‘Einstein frame’’, where, unlike in the original physical formulation (denoted in the literature as the ‘‘Jordan frame’’ [2]), the matter is coupled minimally to gravity. This is achieved by the following (conformal) transformation of the metric tensor and the scalar field $(g_{\mu,\nu}, \phi) \rightarrow (\tilde{g}_{\mu\nu}, \tilde{\phi})$

$$\tilde{g}_{\mu\nu} = 2U g_{\mu\nu}, \quad \left(\frac{d\tilde{\phi}}{d\phi}\right)^2 = \frac{1}{2} \frac{U + 3U'^2}{U^2}. \quad (3.1)$$

Under this change $\tilde{S}[\tilde{g}_{\mu\nu}, \tilde{\phi}] = S[g_{\mu\nu}, \phi]$ and $\tilde{U}(\tilde{\phi}) = 1/2$, thus $\tilde{\phi}$ is indeed minimally coupled to gravity (as required). The explicit relation between $\tilde{\phi}$ and ϕ may be found for all ranges of non-minimal coupling. The metric $\tilde{g}_{\mu\nu}$ can be easily expressed in the FRW form in terms of \tilde{t} and \tilde{a} defined by

$$\tilde{a} = \sqrt{2U}a, \quad d\tilde{t} = \sqrt{2U}dt. \quad (3.2)$$

Effective potential and energy density of $\tilde{\phi}$ transform as follows

$$\tilde{V}(\tilde{\phi}) = \frac{1}{4} \frac{V(\phi(\tilde{\phi}))}{U^2(\phi(\tilde{\phi}))}, \quad \tilde{\rho} = \frac{1}{4U} \dot{\tilde{\phi}}^2 + \tilde{V}. \quad (3.3)$$

The scalar constraint has the standard form of GR minimally coupled to massive scalar field, thus one can directly apply the known procedure of canonical quantization in the LQC framework. Ashtekar-Barbero variables in Einstein frame are of the form of

$$\text{sgn}(\tilde{v})\tilde{v} = \frac{\tilde{a}^3}{2\pi\gamma\sqrt{\Delta}\ell_{Pl}^2}, \quad \tilde{b} = -\gamma\sqrt{\Delta}\frac{1}{\tilde{a}}\frac{d\tilde{a}}{d\tilde{t}}, \quad (3.4)$$

where Δ is the so-called *area gap* [28] which equals $\Delta = 4\pi\gamma\sqrt{3}\ell_{Pl}^2$ [17] and γ is the Barbero-Immirzi parameter [29] equal to $\gamma = 0.2375\dots$ [30]. The Poisson bracket between these variables is $\{\tilde{v}, \tilde{b}\} = 2/\hbar$.⁴

Before proceeding with the quantization let us note that on the classical level we have at our disposal two sets of variables: (v, b, ϕ, π_ϕ) corresponding to the Jordan frame and $(\tilde{v}, \tilde{b}, \tilde{\phi}, \pi_{\tilde{\phi}})$ in the Einstein one. Both sets are related with each other by canonical transformation, thus classically at the level of specified models the selection of either set is simply *a matter of choice*. This may no longer be true, once the perturbations or perturbative quantum corrections are introduced [23, 26]. On the other hand the discrete nature of loop quantization implies that its applications to both frames will most likely lead to *inequivalent* results. The issue of which choice of the frame (in general) should be considered the correct, physical one is under investigation [26], although at present it remains an open question. This issue seems to induce a strong polarization within the cosmological community. Here we do not intend to take sides in this discussion. Instead, we choose one possibility and perform a preliminary study of the model resulting from this choice. Our goal is the initial viability test: verification whether within the minimalistic setting, and under further selection of the quantization method, the model does not lead to immediate contradictions with current cosmological observations. More precisely, we check whether and to what extent the model realizes the operative inflation paradigm (which in turn features the closest agreement with the observations). It often happens in physics that internal consistency of particular theory admits few choices, which next are discriminated on the physical level (via for example agreement with experiments). Our choice here is the assumption that the physical quantities are observed in Jordan frame.

Given the above choice, we introduce one further modification. Usually the selection of the set (the frame) corresponding to the physical, measured quantities is the most natural. In our case that would be the former set. Here however we would like to explore another (somewhat hybrid) approach: to consider the Jordan frame as the one corresponding to observed reality and in which all the measurable quantities should be calculated. However we will think about it as the ‘‘emergent’’ formulation, which should arise from the underlying theory following from the quantization in the Einstein frame. The selection of an Einstein frame as the starting point for quantization has been applied (for other classes of nonminimally coupled fields) for example in [31].

⁴ We use variable \tilde{b} with opposite sign than usual in order to regard \tilde{v} as our configuration variable.

Such approach stems from techniques employed for example in quantum field theory on curved spacetime where the fields are rescaled by a scale factor and the effective field subject to quantization mixes the physical degrees of freedom of the geometry and matter (see for example [32]). In our case it is further motivated by two observations: one of practical, and the other of the philosophical (or rather aesthetic) nature. First, the Einstein frame is a much more natural candidate for quantization. Indeed, in that frame gravity and matter fields are minimally coupled and the gravitational part of the action takes the standard GR form (Einstein-Hilbert action term). Thus, the quantization procedure is natural and well understood. Second, the classical structure (variables) underlying the loop quantization originates from classical GR and encodes its symmetries. Thus, provided that loop quantization is applicable to the considered system at all, Einstein frame is the natural arena for it.

One has to remember, however, that by themselves the above reasons are not sufficient to select the approach as “the right one”. As already stated, we consider it as one of few possibilities. Our goal is to test whether the choices made lead to a viable model worth further studies, or whether it shall be dismissed as unphysical.

The precise implementation of the idea is the following:

- (i) First, we provide the complete quantum description in Einstein frame.
- (ii) Next, the quantum framework is used as the basis for constructing the effective description, used in turn to analyze the dynamical behavior.
- (iii) Finally, the results of dynamics are translated to the “physical” Jordan frame.

IV. LOOP QUANTIZATION

As discussed above, we quantize the system in Einstein frame, choosing the polymer representation for the geometry degrees of freedom and the Schrödinger one for the matter ones. Thus, the quantization procedure is a full analogy of the one applied to the FRW cosmology with minimally coupled massless scalar field in [28]. Such a “hybrid” approach can in principle be considered inconsistent, as geometry and matter are treated differently. Indeed, the strictly systematic procedure should involve the polymeric quantization of all the degrees of freedom. In full Loop Quantum Gravity the systematic polymeric quantization of the scalar field is known [33]. In context of the symmetry-reduced models it has also been studied [34, 35]. In particular, the analysis of the massless scalar field in FRW universe performed in [35] has shown that the dynamics of such system is *identical* to the one of the system where the scalar field has been quantized a la Schrödinger. However, the polymer quantization of the scalar field admits a critical difference in comparison to the geometry. The latter admits a precisely defined “loop scale” – essentially an energy scale at which quantum gravity effects become significant [28]. Such precise scale follows directly from the fact that the first nonzero eigenvalue of the LQG area operator is well distinct from zero. In the case of the scalar field, the operator playing an analogous role has eigenvalues arbitrarily close to zero [36]. As a consequence, the “loop scale” for the scalar field cannot be determined the way it is for the geometry. Furthermore, the spectral structure indicates that in such case taking the continuous limit within the loop quantization may be the correct approach, thus effectively leading to Schrödinger quantization. The issue is however still under study. For this reason, and due to the preliminary nature of our studies, we follow the “hybrid approach”: polymeric quantum geometry and Schrödinger quantum matter. At this stage of the investigation such approach has the further advantage of the ability to directly compare our results with the existing LQC literature.

Let us now outline briefly the procedure itself. To start with, we employ (the initial part of) the Dirac program, first quantizing the system on the kinematical level (ignoring the constraint). The resulting kinematical Hilbert space, \mathcal{H}_{kin} , is of the form

$$\mathcal{H}_{\text{kin}} = \mathcal{H}_{\text{gr}} \otimes \mathcal{H}_{\phi}, \quad \mathcal{H}_{\text{gr}} = L^2(\bar{\mathbb{R}}, d\mu_{\text{Bohr}}), \quad \mathcal{H}_{\phi} = L^2(\mathbb{R}, d\phi), \quad (4.1)$$

where $\bar{\mathbb{R}}$ is the Bohr compactification of the real line. A convenient basis of \mathcal{H}_{gr} is formed by the eigenstates of the oriented volume operator $\hat{V} \equiv \hat{a}^3$

$$\hat{V}|\tilde{v}\rangle = 2\pi\gamma\sqrt{\Delta}\ell_{\text{Pl}}^2\tilde{v}|\tilde{v}\rangle =: \alpha|\tilde{v}\rangle, \quad (4.2)$$

where $|\tilde{v}\rangle$ is eigenstate of operator \hat{v} with eigenvalue \tilde{v} . They are orthonormal with respect to Kronecker delta, that is $\langle\tilde{v}|\tilde{v}'\rangle = \delta_{\tilde{v},\tilde{v}'}$. On the other hand, the basis of \mathcal{H}_{ϕ} is provided by the generalized eigenstates $(\tilde{\phi}|$ of the operator $\hat{\phi}$ – a quantum counterpart of the field value $\tilde{\phi}$:

$$\forall\chi \in \mathcal{H}_{\phi} \quad (\tilde{\phi}|\hat{\phi} - \tilde{\phi}\hat{I}|\chi\rangle = 0. \quad (4.3)$$

At this point a short comment regarding the exact physical meaning of the quantity \tilde{V} is in order. In order to obtain a meaningful canonical description of an isotropic model with noncompact spatial slices (which is the case here), one introduces into the theory an infrared regulator – some fiducial cell \mathcal{V} constant in comoving coordinates. The quantity $\tilde{V} = \tilde{a}^3$ here corresponds exactly to the (oriented) volume of that cell. Of course, one has to remember that in order to obtain consistent description one has to make sure that the theory admits a well defined regulator-removal limit.

Given \mathcal{H}_{kin} , we now select the basic operators defined on some dense domain of it. Two of them are the operators \hat{v} and $\hat{\phi}$ (4.2, 4.3). The remaining two are the unit shift operator \hat{N} and the scalar field momentum $\hat{\pi}_{\tilde{\phi}}$:

$$\hat{N}|\tilde{v}\rangle = |\tilde{v} + 1\rangle, \quad \hat{\pi}_{\tilde{\phi}} = i\hbar\partial_{\tilde{\phi}}. \quad (4.4)$$

The pair \hat{v}, \hat{N} is the equivalent of the operators of quantum flux and holonomy in full LQG, where the holonomy-flux algebra provides the basis for quantization [12]. In particular, \hat{v} represents (the power of) the flux across the unit surface (in comoving coordinates), whereas \hat{N} the holonomy along straight line [37].

The set $(\hat{v}, \hat{N}, \hat{\phi}, \hat{\pi}_{\tilde{\phi}})$ is sufficient to construct the quantum counterpart of the Hamiltonian constraint – the next step in Dirac program. The details of its construction are presented in [28]. However, here we choose a bit different and more convenient symmetric factor ordering, the one used in [38]. The resulting operator is

$$\hat{\mathbf{H}} = \hat{\mathbf{H}}_{\text{gr}} \otimes \mathbb{I}_{\phi} + \hat{\mathbf{H}}_{\phi}, \quad \hat{\mathbf{H}}_{\text{gr}} = \frac{3\pi G}{8\alpha} \sqrt{|\tilde{v}|} (\hat{N}^2 - \hat{N}^{-2})^2 \sqrt{|\tilde{v}|}, \quad (4.5a)$$

$$\hat{\mathbf{H}}_{\phi} = \frac{1}{2\alpha} \widehat{|\tilde{v}|^{-1}} \pi_{\tilde{\phi}}^2 + \frac{\alpha}{\hbar} |\tilde{v}| \tilde{V}(\tilde{\phi}), \quad (4.5b)$$

where α is defined via (4.2) and $\tilde{V}(\tilde{\phi})$ is the effective potential given by (3.3).

Having at our disposal both \mathcal{H}_{kin} and the quantum constraint $\hat{\mathbf{H}}$ we can complete the Dirac program, constructing the physical Hilbert space (out of states annihilated by $\hat{\mathbf{H}}$) via group-averaging procedure [39], and introducing the family of unitarily related observables to capture nontrivial information about the evolution of the described system. Such observables can be again constructed out of self-adjoint operators on \mathcal{H}_{kin} (kinematical observables) via group averaging. In generic situations, however, the form of the resulting physical observables is very different than the original kinematical ones. Therefore, to obtain a technically manageable theory, one usually resorts to the so-called *deparametrization*, introducing into the system a suitable matter field and using it as an internal clock. This is exactly the method originally used in [28].

One such deparametrization, particularly successful in full LQG, has been introduced in [40]. There, the time variable is provided by irrotational dust (see [41] for studies of dust frames and [42] for application of *full* dust frame to LQG). Then, the synthesis of three elements (the specific matter field, the fixing of the time gauge provided by the proper time of dust “particles”, and the diffeomorphism-invariant formalism of standard LQG) allow to build a technically manageable completion of gravity quantization program. Its reduction to isotropic cosmology has been presented in [38]. Its main properties are: (i) the Hamiltonian constraint becomes true Hamiltonian, (ii) the kinematical Hilbert space \mathcal{H}_{kin} becomes (precisely) the physical one, so do the kinematical observables, and (iii) the evolution of the physical state is described by time-dependent Schrödinger equation

$$-i\hbar\partial_{\tilde{t}}\Psi(\tilde{v}, \tilde{\phi}) = \hat{\mathbf{H}}\Psi(\tilde{v}, \tilde{\phi}), \quad (4.6)$$

where the time \tilde{t} provided by the gauge choice agrees with the cosmic time and the Hamiltonian $\hat{\mathbf{H}}$ (in our case given by (4.5)) is self-adjoint for any system of gravity coupled to non-exotic matter [43]. This quantum description provides an excellent basis for further analysis of the dynamics. It can be performed on the genuine quantum level, although in this paper we will employ the so called *effective description* which will be introduced in the next section.

In order to describe the dynamics we select the following set of observables, convenient in cosmology: scaled quantum volume $|\hat{v}|$, operator $\widehat{\sin(\tilde{b})} := (i/2)[\hat{N}^2 - \hat{N}^{-2}]$, field $\hat{\phi}$ and its momentum $\hat{\pi}_{\tilde{\phi}}$. All these operators, being originally kinematical observables in irrotational dust deparametrization automatically become physical.

Another observable especially relevant for cosmology and in particular for our further studies is an operator corresponding to Hubble parameter. It takes the form:

$$\hat{H} = -\frac{1}{4i\gamma\sqrt{\Delta}}[\hat{N}^4 - \hat{N}^{-4}]. \quad (4.7)$$

At this point it is worth noting that the dust field, although convenient, is not the only possible choice of the internal time. One alternative, viable in the cosmological context is the choice of additional – massless scalar field.

Such field has been used exactly in the pioneering work [28] and is in fact the most popular choice of clock in LQC. Its application to the full theory is well defined (as variation of the formalism of [44]) at least formally, however the complications related with the properties of the scalar field keep its application to non-cosmological settings beyond current technical reach. In the homogeneous cosmology context it is manageable, although not free from (minor) technical difficulties, such as: (i) evolution is provided by Klein-Gordon equation rather than Schrödinger one, (ii) in presence of any non-negative scalar field potential the Hamiltonian loses self-adjointness, and (iii) the physical Hilbert space is a proper subspace of \mathcal{H}_{kin} and its identification requires explicit knowledge of spectral properties of $\hat{\mathbf{H}}$. We discuss this formalism in more detail in appendix A.

V. EFFECTIVE THEORY

At this point we have at our disposal the physical Hilbert space, time, true Hamiltonian operator and the set of physical quantum observables. These components are sufficient to systematically study the dynamics of our system. The analysis on the genuine quantum level can be performed by the methods of [45]. However, since the aim of this paper is to obtain maximally complete picture of the semiclassical sector of the theory we resort to effective methods, leaving the verification of the results against the genuine quantum ones to future work. To arrive to such effective description, we employ the method introduced in [46] (allowing in principle to account for arbitrary order quantum corrections, see e.g. [47]) in its 0th order. In this order the resulting set of equations of motion is equivalent to the one provided by heuristic methods of the so called *effective dynamics of LQC* [48]. Its comparison against the genuine quantum dynamics in many LQC systems [28, 49–51] has shown that it mimics the full quantum evolution to high level of accuracy. Furthermore, in some cases this result has been confirmed analytically [52].

Technically, the method reduces to replacing the basic operators in quantum Hamiltonian by their expectation values evaluated on the semiclassical (sharply peaked) states⁵. In our case, this is

$$\hat{v}^n \mapsto \langle \hat{v} \rangle^n, \quad \hat{N} \mapsto \langle \hat{N} \rangle e^{i\tilde{b}/2}, \quad (5.1)$$

Applying this mapping to (4.5), we get the following “classical” effective Hamiltonian

$$\mathbf{H}_{\text{eff}} = -\frac{3\pi G}{2\alpha} |\tilde{v}| \sin^2(\tilde{b}) + \frac{\pi_{\tilde{\phi}}^2}{2\alpha |\tilde{v}|} + \frac{\alpha |\tilde{v}|}{\hbar} \tilde{V}(\tilde{\phi}) = E_{\text{eff}}. \quad (5.2)$$

where E_{eff} is the energy of the dust clock field. The full set of the effective equations of motion is then provided by Hamilton’s equations

$$\frac{d\tilde{v}}{d\tilde{t}} = -\frac{6\pi G}{\alpha \hbar} |\tilde{v}| \sin(\tilde{b}) \cos(\tilde{b}) \quad \frac{d\tilde{b}}{d\tilde{t}} = \frac{3\pi G}{\alpha \hbar} \sin^2(\tilde{b}) + \frac{\pi_{\tilde{\phi}}^2}{\alpha \hbar \tilde{v}^2} - \frac{2\alpha}{\hbar^2} \tilde{V} \quad (5.3a)$$

$$\frac{d\tilde{\phi}}{d\tilde{t}} = \frac{\pi_{\tilde{\phi}}}{\alpha |\tilde{v}|} \quad \frac{d\pi_{\tilde{\phi}}}{d\tilde{t}} = -\frac{\alpha |\tilde{v}|}{\hbar} \frac{\partial \tilde{V}}{\partial \tilde{\phi}} \quad (5.3b)$$

In order to eliminate the effects of the dust field on the dynamics, we set

$$E_{\text{eff}} = 0, \quad (5.4)$$

thus reducing the presence of dust to a “dust vacuum”. Under this condition the set of equations of motion (5.3a) and (5.2, 5.4) becomes equivalent to the following set

$$3\tilde{H}^2 = 8\pi G \tilde{\rho} \left(1 - \frac{\tilde{\rho}}{\rho_{cr}}\right), \quad \frac{d\tilde{H}}{d\tilde{t}} = -4\pi G (\tilde{\rho} + \tilde{P}) \left(1 - 2\frac{\tilde{\rho}}{\rho_{cr}}\right), \quad (5.5)$$

where $d\tilde{v}/d\tilde{t} = 3\tilde{v}\tilde{H}$ and $\rho_{cr} = 3/8\pi G \Delta \gamma^2$. The Big Bounce in Einstein frame appears for $\tilde{\rho} = \rho_{cr}$.

It is worth noting that (5.5) can be converted to Jordan frame via (3.1), giving

$$6UH^2 + 6U'H\dot{\phi} + \dot{\phi}^2 \frac{3U'^2}{2U} = 8\pi G \left(\rho + \dot{\phi}^2 \frac{3U'^2}{2U}\right) \left(1 - \frac{1}{4U^2 \rho_{cr}} \left(\rho + \dot{\phi}^2 \frac{3U'^2}{2U}\right)\right), \quad (5.6a)$$

$$\dot{H} + H \frac{U'\dot{\phi}}{U} + \dot{\phi}^2 \frac{2UU'' - 3U'^2}{4U^2} = -8\pi G \dot{\phi}^2 \frac{U + 3U'^2}{4U^2} \left(1 - \frac{1}{\rho_{cr}} \left(\dot{\phi}^2 \frac{U + 3U'^2}{4U^3} + \frac{V}{2U^2}\right)\right). \quad (5.6b)$$

⁵ There we assume implicitly, that there exists a sufficiently large space of such states. Verification of this assumption requires testing the dynamics on the genuine quantum level.

Note that for $\xi\phi^2 \gg 1$, unlike in the case of LQC with minimal coupling, at the moment of the Bounce we have $\rho \gg \rho_{cr}$.

The equation of motion for ϕ is of the form (2.4a): surprisingly, the effective rolling force of the scalar field is not changed by the LQC correction, and the LQC correction does not influence the classical equation of motion for $\tilde{\phi}$, which (after the substitution of $\tilde{\phi} = \tilde{\phi}(\phi)$) gives eq. (2.8).

VI. THE ANALYSIS OF THE DYNAMICS

The set of equations of motion in the Einstein frame (5.3) allows in principle to evaluate the time evolution of the canonical data $(\tilde{v}, \tilde{b}, \tilde{\phi}, \pi_{\tilde{\phi}})$ up to the caveat that the form of $\phi(\tilde{\phi})$ is needed to specify $\tilde{V}(\tilde{\phi})$. This dependence is provided through the differential relation (3.1). Therefore, for the sake of precision, it is much more convenient to formulate and integrate the mixed set of equations of motion for the variables $(\tilde{v}, \tilde{b}, \phi, \pi_{\tilde{\phi}})$, where the equation for $d\phi/dt$ follows from (5.3b) and (3.1). This set allows to determine all the relevant physical parameters. For technical reasons (faster evolution), it is more convenient to evolve the system with respect to the “physical” time t of the Jordan frame. Using (5.3), we arrive to the final set of the evolution equations:

$$\frac{d\tilde{v}}{dt} = -\frac{6\pi G}{\alpha\hbar} \sqrt{2U(\phi)} |\tilde{v}| \sin(\tilde{b}) \cos(\tilde{b}) \quad \frac{d\tilde{b}}{dt} = \sqrt{2U(\phi)} \left[\frac{3\pi G}{\alpha\hbar} \sin^2(\tilde{b}) + \frac{\pi_{\tilde{\phi}}^2}{\alpha\hbar\tilde{v}^2} - \frac{2\alpha}{\hbar^2} \tilde{V} \right] \quad (6.1a)$$

$$\frac{d\phi}{dt} = \sqrt{\frac{4U^3(\phi)}{U(\phi) + 3U'^2(\phi)}} \frac{\pi_{\tilde{\phi}}}{\alpha|\tilde{v}|} \quad \frac{d\pi_{\tilde{\phi}}}{dt} = -\frac{\alpha|\tilde{v}|}{\hbar} \sqrt{\frac{4U^3(\phi)}{U(\phi) + 3U'^2(\phi)}} \frac{\partial\tilde{V}}{\partial\phi}. \quad (6.1b)$$

In order to specify the initial conditions for the time evolution, we exploit the fact that each physical trajectory has a distinguished point, namely the big bounce in the Einstein frame (at which $\tilde{b} = \pi/2$). We chose it as our “initial point”, setting $t = 0$ there and evolving the initial data (set there) both forward and backward in time. Since the set (6.1) is homogeneous in \tilde{v} ,⁶ we have the freedom in choosing its initial value. We set it to 1. Having the geometry degrees of freedom set, we fix the scalar field momentum $\pi_{\tilde{\phi}}$ as the function $\pi_{\tilde{\phi}}(\tilde{v}, \tilde{b}, \phi, E_{\text{eff}})$ using the Hamiltonian (5.2). To eliminate the influence of the dust “clock” field on the dynamics we further set its energy E_{eff} to zero. As a consequence we have at our disposal a 1-parameter family of initial data ($t = 0, \tilde{v} = 1, \tilde{b} = \pi/2, \phi_{\text{in}}, \pi_{\tilde{\phi}} = \pi_{\tilde{\phi}}(\tilde{v} = 1, \tilde{b} = \pi/2, \phi_{\text{in}}, E_{\text{eff}} = 0)$) parametrized by the value ϕ_{in} of the scalar field ϕ at the bounce point in the Einstein frame.

These initial data, supplied (and determined) by the set of constants ξ, λ , was then evolved using the fifth order adaptive Runge-Kutta (Cash-Carp) method using the effective dynamics module of the Numerical LQC library developed by T. Pawłowski and J. Olmedo. The raw results of the simulations were next postprocessed with the use of *Mathematica* and *gnuplot* software.

In actual simulations the value of λ was set to 1/2, which is the same order of magnitude as in the Standard Model. Due to the running of the coupling constant one cannot predict the precise value of λ around the Planck scale. However recent results from ATLAS and CMS [9, 10] suggest that λ shall not be too big, since the mass of the Higgs is close to the minimal allowed value which does not violate electroweak vacuum. Thus, the value of λ assumed by us is realistic.

The relation between coupling constants ξ and λ is given by the normalization of primordial inhomogeneities, which gives $\xi = 47000\sqrt{\lambda}$. However, to confirm the robustness of the results and further analyze the qualitative behavior of the system, several different values have been considered: the sequence of lower values $\xi_n = \{4.7 \times 10^n \sqrt{\lambda}; n = 0, \dots, 3\}$. To test the wide range of trajectories the initial scalar field values were chosen from the interval $\phi_{\text{in}} \in (-10\xi^{-1/2}, 10\xi^{-1/2})$. For most simulations we selected 20 initial points distributed uniformly within this interval. These initial data have been next evolved till the time $t_{\text{fin}} = 2 \times 10^3, \dots, 10^5$ depending on the simulation (and, in particular, on the constant ξ). The results of these simulations are discussed in the next section.

VII. THE RESULTS

The results of our studies can be summarized in the following set of points:

⁶ One needs to remember that \tilde{v} encodes the information about the physical volume of the chosen region of spacetime, whose choice for noncompact spatial topology of the universe is arbitrary.

- In the (underlying) Einstein frame we observe the standard for LQC picture of a single bounce separating contracting and expanding epochs of the universe evolution. The “bare” matter energy density $\bar{\rho}$ and Hubble parameter are bounded by their respective critical values $\rho_c \approx 0.41\rho_{\text{Pl}}$ and $H_c \approx 1.3\ell_{\text{Pl}}^{-1}$.
- In the Jordan frame, here conjectured to represent the observed dynamics, the standard bounce paradigm is slightly changed. The single large energy density epoch still separates two long epochs of contraction and expansion. The process of the bounce itself is however modified: the evolution of the scale factor features the so called “mexican hat” shape (see Fig. 4) – the sequence of bounce, ultrarapid nonadiabatic expansion ending with recollapse, similar nonadiabatic epoch of contraction and the final (second) bounce, after which the universe expands to the classical regime (see also Fig. 3 for the Hubble parameter evolution). The time between the bounces is of the order of Planck time.
- Outside of the “mexican hat bounce” the dynamical trajectory approaches quickly the one predicted by GR. In particular in the future of the bounce the value of the field ϕ grows to certain (depending on the trajectory) maximal value ϕ_{infl} at which point the slow roll inflation starts. Due to the time symmetry of the equations of motion the inflation after the bounce is accompanied by the “slow roll” deflation before it. The initial Hubble parameter at the onset of inflation is proportional to ϕ_{infl} (see Fig. 2(a)).
- The number of e-foldings during the inflation is estimated to be $N_+ \simeq 3/16\xi\phi_{\text{infl}}^2$ and for the physical value of $\xi \approx 4.7 \cdot 10^4$ exceeds 60 within all the studied range of initial data (see Fig. 2(b)). The same estimate holds for the deflation: $N_- \simeq 3/16\xi\phi_{\text{def}}^2$, where ϕ_{def} is the minimal value of the field (reached before the bounce).
- Within the precision of our estimates, the product N_+N_- of the e-foldings during inflation and deflation does not depend on the initial data. It is the function of ξ and λ only, in particular growing with ξ . For the selected values of ξ, λ it equals $N_+N_- = [4.4 \cdot 10^3]^2$ (see Fig. 2(b)). This also implies that to have an inflation with $N < 60$, there must be a deflation with $N > 10^6$. This is an extremely asymmetric situation, and therefore highly unlikely at least on the intuitive level: we thus expect that the inflation with $N > 60$ is extremely probable - with much higher probability than in the case of the standard chaotic inflation.
- At the late time each trajectory reaches the standard inflationary attractor and the reheating (see Fig. 5 for the illustration on the example of the unphysical model corresponding to $\xi = 47\sqrt{\lambda}$).

VIII. CONCLUSIONS

We investigated the model of non-minimally coupled scalar field coupled to gravity via additional term in the Lagrangian density: $\frac{1}{2}\xi\phi^2R$ and with potential $\frac{1}{4}\lambda\phi^4$. This system has been studied via effective dynamics methods within loop quantum cosmology framework. In the process of constructing the treatment we implemented the idea where the so-called Jordan frame represents the observed (physical) dynamics, however it is an emergent framework coming from underlying one represented by Einstein frame. The studies have shown that, similarly to other models within LQC, the high density region connects two semiclassical branches of the universe: contracting and expanding. However the process of the bounce itself is modified, featuring the “mexican hat” shape of the scale evolution with highly non-adiabatic epoch of expansion→contraction between two bounces. The expanding epoch features the slow roll inflation whose length for all the investigated trajectories exceeds 60 e-foldings. These results, although solid within the specified model, cannot be treated as final due to the model origin and its limitations. As we discussed in sec. III, in the process of constructing the model we have made a selection of several alternatives in two aspects: which frame is the “observed” one and which is the correct starting point for quantization. The choices are not distinguished by any physical considerations. We simply tested one of few possible constructions in order to check whether it leads to unphysical results or, conversely, it is worth further investigation.

Let us now discuss the limitations: First, the quantization procedure applied here assumes the role of Jordan frame as the observed one and the Einstein frame as the underlying (somehow more fundamental) one. Such approach raises a (natural for non-minimally coupled systems) concern, that the description may admit a Lorentz symmetry violation, which in principle could imply disagreement with the cosmological observations (for example, through the structure of the primordial gravitational waves). To the best of our knowledge there does not exist any definite result indicating that this would be the case but the issued in itself remains still open.

One also needs to remember that the above approach is just one of two possible in this case: quantization in Einstein and Jordan frame. Their quantization, especially the loop one may a priori lead to different dynamical results. At present there is no definite argument known which would select one of them as physical. In our studies we have taken the “trial and error” approach performing the “physical viability” test, i.e. checking whether the choice of the particular

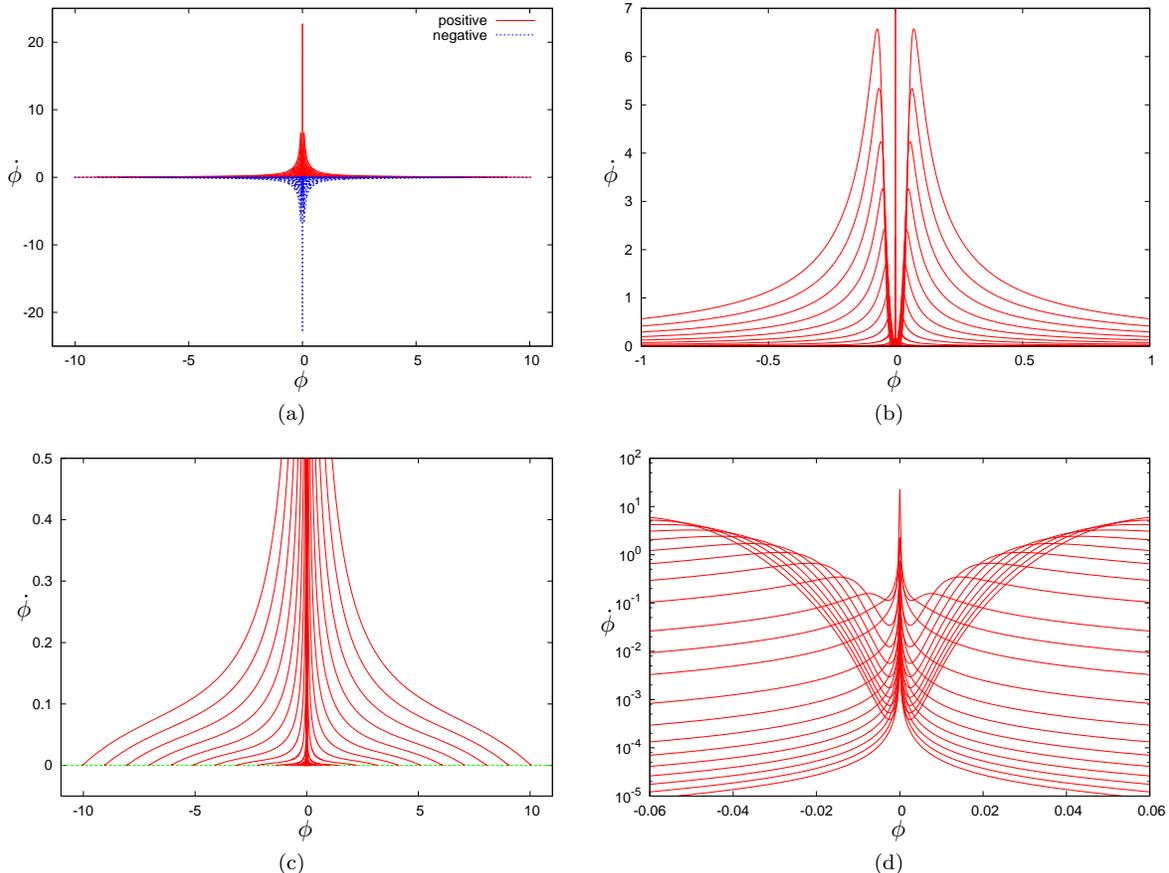


FIG. 1. Global view 1(a) and the zoom into particular sectors of the phase portrait with respect to matter degrees of freedom for the physical case of $\xi = 47000\sqrt{\lambda}$. In 1(b) we zoom the region around the bounce in the Einstein frame. Figure 1(c) shows the trajectories at the onset of inflation (at $\dot{\phi} = 0$), providing the initial conditions for inflation. We do not show the attractor trajectory, as the length of inflation exceeds the technical (time) limits of our numerical simulations. 1(d) shows the same sector as 1(b) in the logarithmic scale to visualize the behavior of trajectories for small $\dot{\phi}$.

frame would lead to immediate disagreements with known properties of the universe (and should thus be discarded) or, on the contrary, would give a promising point of departure for the model consistent with observations. In this paper we have selected for our studies Einstein frame, as for this case we have at our disposal the complete framework in context of full LQG. In consequence, the existing techniques of LQC could be applied directly. In the remaining case one needs to adapt the existing full LQG framework. This is a work currently in progress [53]. At present, it is already known that the modification of the formalism is essentially restricted to the fact of the constraints being of a different form (than the “original” LQG one), as expressed in terms of the adapted Ashtekar-Barbero variables. There is no indication of any conceptual problems preventing one from completing this framework. This expectation is further supported by the existing results in context of $f(R)$ and Brans-Dicke theories [54]. Of course, in context of the homogeneous LQC the necessary adaptation is much more straightforward. Early results of the LQC quantisation in Jordan frame suggest significant differences of the evolution of space-time around the bounce as well as different scale of the bounce in Jordan frame. Full analysis of the model considered here and comparison with the Einstein frame quantisation is the goal of the future work.

Furthermore, the chosen quantization procedure in its exact form as specified in the paragraph above and in Sect. IV is strictly tailored to the situations where the gravitational part of the Hamiltonian can be expressed in the form where matter is minimally coupled to gravity. However, such assumption cannot be satisfied for a vector field non-minimally coupled to gravity (like models with vector inflation [4]), as the transformation described in the eq. (3.1) would still leave non-minimal coupling terms. Nonetheless, one *can* achieve the properties of the Einstein frame relevant for loop quantization of the geometry. Namely, the frame can be transformed to the one where the gravitational part of the action has the standard Einstein-Hilbert form. This is sufficient to apply standard loop techniques in their present form. In such case however the matter field would be still nonminimally coupled to gravity, which would require to

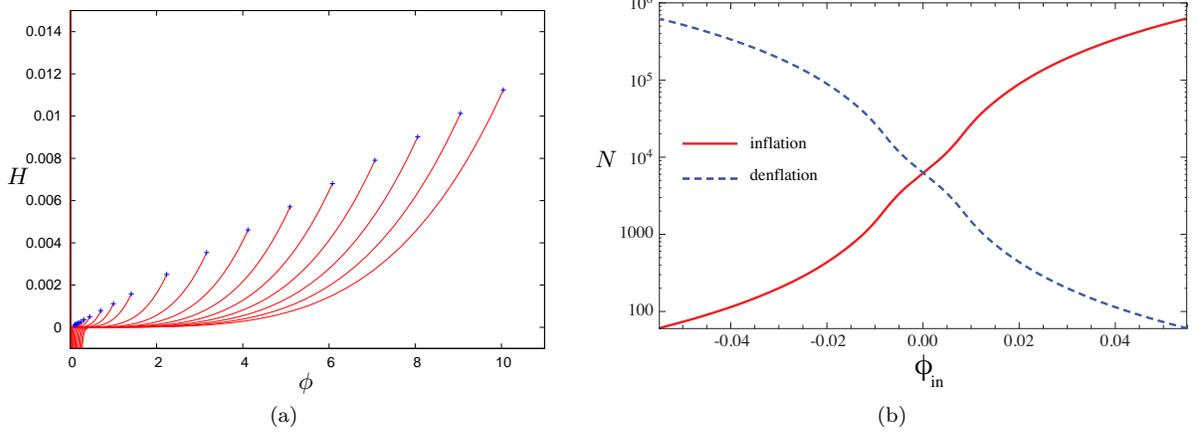


FIG. 2. 2(a) Projection of the phase portrait onto the ϕ - H plane. The trajectories reach the onset of inflation (marked by blue crosses) which points lie on a straight line (as expected in the strong non-minimal coupling case, where $H \simeq \pm\sqrt{\lambda/12\xi}|\phi|$). 2(b) shows the number of e -foldings during the slow-roll inflation after the bounces (red line) and the deflation before the bounces (blue line) as a function of initial value of the field (labeling the trajectories). Notice that even the trajectories with very high time reversal asymmetry (considered to be unlikely) give more than 60 e -foldings during inflation.

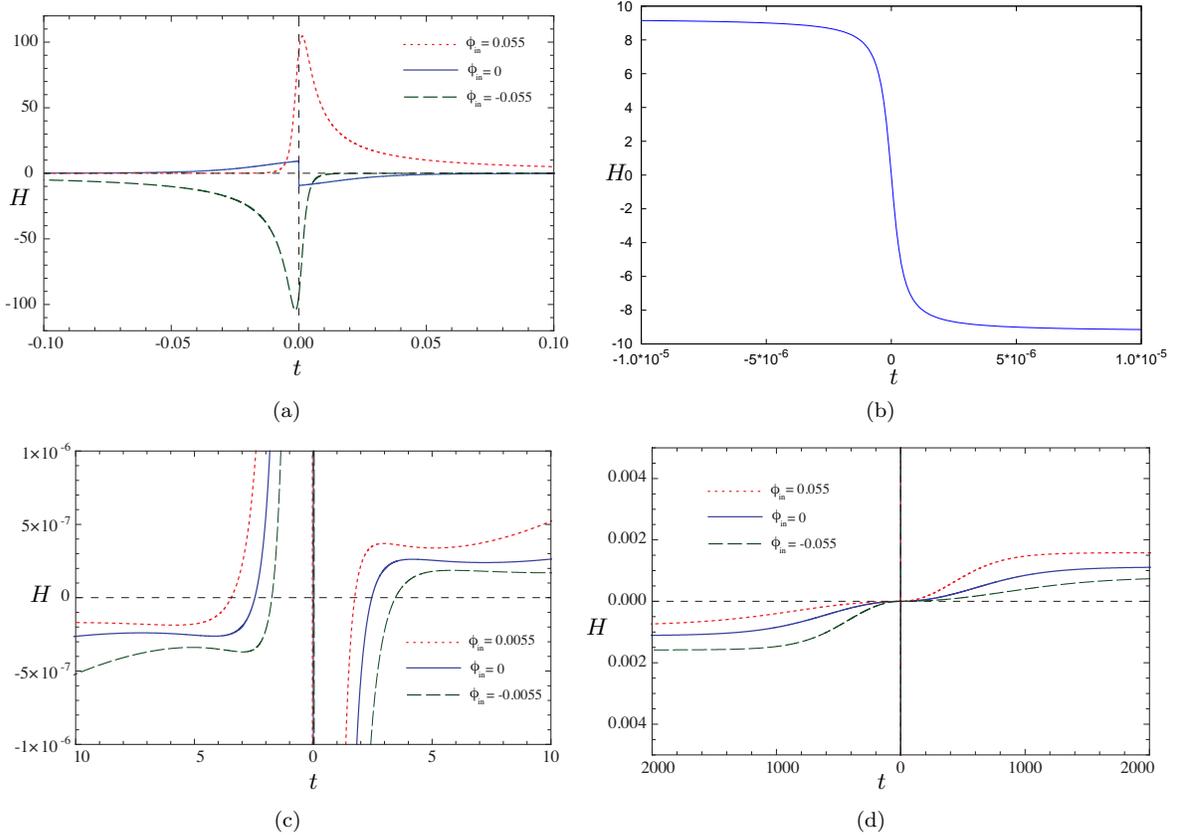


FIG. 3. Evolution of the Hubble parameter as a function of time (in Planck units) for the symmetric trajectory ($\phi_{\text{in}} = 0$) and for two non-symmetric ones. Fig. 3(a) shows the general view around the epoch of high energy density. In 3(b) we zoom around $t = 0$ for the symmetric trajectory only (with the recollapse at $t = 0$), to show that the transition is in fact smooth. 3(c) visualizes two bounces in Jordan frame. 3(d) shows the regions of the onset of inflation and the end of deflation, where H is approximately constant.

use for the matter the quantization schemes of non-canonical kinetic terms following from QFT (see for example [55]).

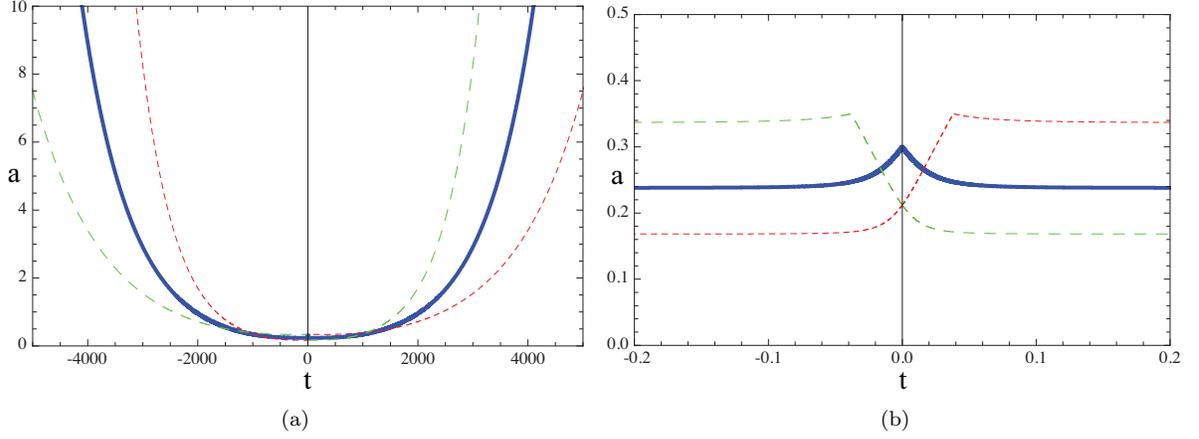


FIG. 4. The evolution of the scale factor for the symmetric trajectory and for two non-symmetric ones ($\phi_{\text{in}} = \pm 0.0055$) 4(a) and its close-up around $t = 0$ 4(b) showing the characteristic “mexican hat” shape with two bounces and recollapse between them. Note that for non-symmetric trajectories the “tip of the hat” (i.e., the moment of recollapse) is shifted in time and less evident.

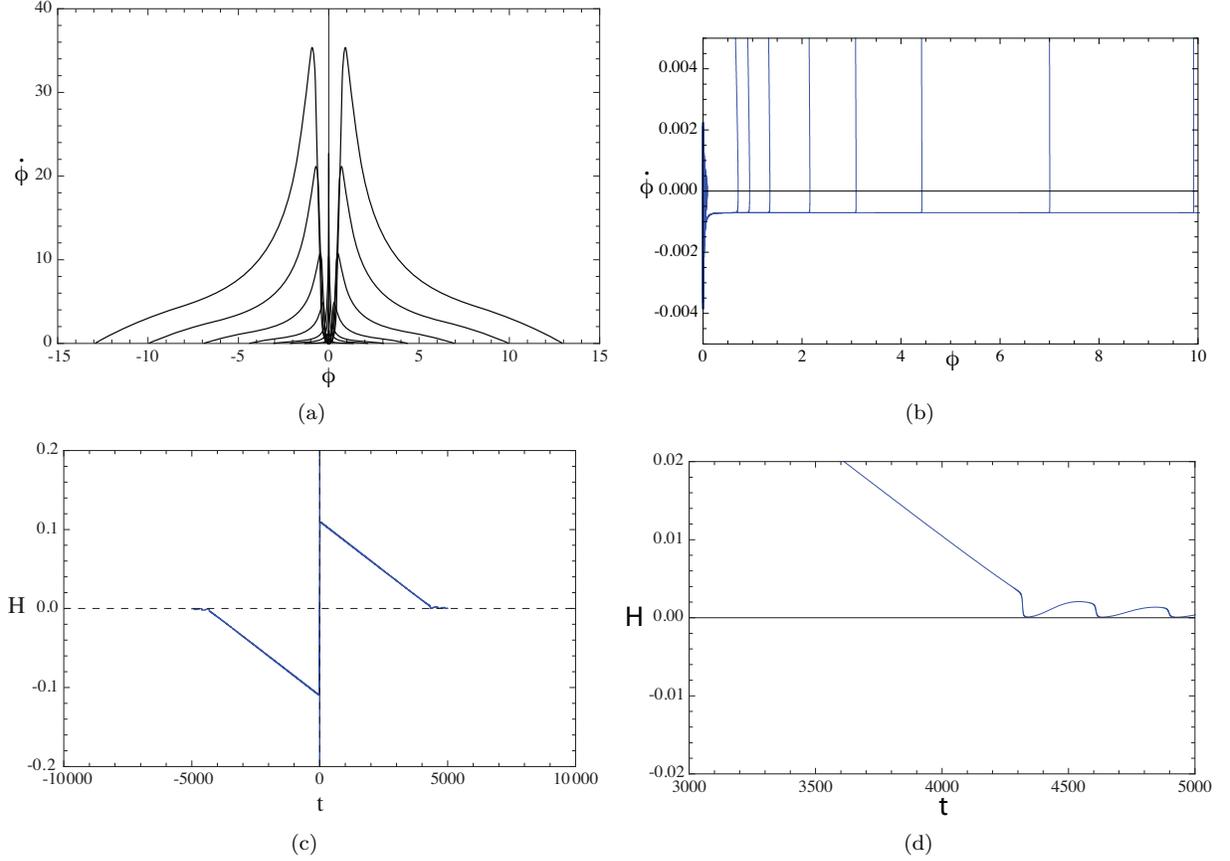


FIG. 5. Phase space (matter sector: ϕ - $\dot{\phi}$ plane) and evolution of Hubble parameter for the $\xi = 47\sqrt{\lambda}$ toy model. For such a small value of the coupling we are able to evolve the system through the whole inflation. Fig. 5(a) shows the global view of the $\dot{\phi}$ half. 5(b) shows the approach of the trajectories towards the attractor (ending in the reheating at $\dot{\phi} \sim \sqrt{\lambda}\phi^2$). In 5(c) we present the time evolution of the Hubble parameter during the inflation/deflation epoch. 5(d) is a close-up of the same evolution around reheating. The qualitative features demonstrated here are expected to be also present in the realistic $\xi = 47000\sqrt{\lambda}$ case.

This problem (as well as the above solution to it) is present even if a non-minimally coupled vector field is subdominant, i.e. when the presence of a vector field does not break isotropy of the background metric tensor. The same applies to any multi-inflationary scenarios with at least two fields non-minimally coupled to gravity.

One has also to remember that the results presented in this paper have been obtained via the 0th order effective dynamics. This choice of methodology is motivated on the one hand by the reliability of the method itself proven for other models of LQC and, on the other hand, by the aim of the study: verifying the robustness of sufficiently long inflation in the model considered (which in turn required probing maximally wide region of the space of solutions). However, the reported results can be treated as preliminary only, since the state-dependent parameters may affect the dynamics especially in the strongly nonadiabatic epoch between the bounces. Therefore, the effective method has to be confirmed by a higher order effective treatment of [46] and especially by the studies of the dynamics on the genuine quantum level within the framework of [38] (the latter in particular to determine the viable cutoff of the effective treatment order). These studies will be performed in future work.

Finally, let us note that the modification of the dynamics in the high energy epoch may also affect the structure of the inhomogeneities in the universe. Within the treatment explored in this paper any classical perturbative framework should be constructed (and then subsequently quantized) in the Einstein frame generalized as discussed several paragraphs earlier. Then, (in particular) the possible formation of shock waves in the strongly nonadiabatic epoch between bounces may in principle affect the structure formation in the expanding universe. Addressing these issues requires however extending the simple isotropic formalism used in this paper to inhomogeneous situations and further comparing the results with the analogous ones obtained in the Jordan frame directly. The first step in the latter is the formulation of a well defined canonical formalism (in particular the adapted Ashtekar-Barbero variables) directly in the Jordan frame, followed next by the quantization within LQG framework. Then, an application of recent developments in the deparametrization techniques of LQG [40] will allow to unambiguously control the dynamical sector of the full theory.

This in turn will allow to construct a precise perturbative framework (in both the generalization of the Einstein frame and the Jordan frame for comparizon). Methods of building such framework are already available in the context of LQC. They are: the *hybrid quantization* [56], strictly implementing the unitary evolution, or *Quantum Field Theory on Quantum Cosmological Spacetime* [57], already showing some preliminary successes in determining the primordial perturbations [58]. Applying these tools to the scenario studied here will ultimately allow to test its consistency with CMB observations and identify possible effects characteristic for it.

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Appendix A: Deparametrization via massless scalar field

One of the steps performed in order to arrive to an effective description of the considered system in Sec. V was the introduction of the dust matter field and next the deparametrization of the system with respect to it. While this particular choice of the clock allows the full formal control over each step of the construction of the effective description, it is by no means the only one possible. Indeed, deparametrization can be performed (at the cost of a limited loss of precision) with respect to other matter fields of sufficiently good properties, for example the massless scalar considered in the original LQC works [28] or the (appropriately tailored) population of Maxwell fields [59]. As long as we restrict the expansion to the 0th order and assume vanishing mean energy of the clock field, the formalism leads to exactly the same equation of motion (5.3) as in the case of dust clock. In this appendix we briefly outline the construction of the effective description with use of the massless scalar field. The exact same procedure can be applied to Maxwell fields of [59].

Our starting point is the modification of the classical Hamiltonian constraint in the Einstein frame, namely adding to it the massless scalar field term:

$$\mathbf{H} \rightarrow \mathbf{H}' = \mathbf{H} + \mathbf{H}_\varphi, \quad \mathbf{H}_\varphi = \frac{p_\varphi^2}{2\alpha|v|}, \quad (\text{A1})$$

where p_φ is the canonical momentum of the clock field φ and the variable v (and the constant α) is defined via eq. (4.2). This constraint is next deparametrized with respect to φ^7 , in effect being brought to the form

$$p_\varphi^2 = \Theta = -2\alpha|v|\mathbf{H}, \quad (\text{A2})$$

which in turn can be understood of as representing the free system evolving with respect to φ . Applying polymer quantization as in Sec. IV (see [28] for further information) we arrive to the generalized Klein-Gordon equation

$$-\partial_\varphi^2 \Psi(v, \phi) = \hat{\Theta} \Psi(v, \phi), \quad \hat{\Theta} = -2\alpha :|\hat{v}|\hat{\mathbf{H}}: , \quad (\text{A3})$$

where $: \cdot :$ means the symmetric ordering. Action of $\hat{\Theta}$ on a dense domain in \mathcal{H}_{kin} reads (following [50] for its gravitational part)

$$\hat{\Theta} = \hat{\Theta}_{\text{gr}} \otimes \mathbb{I}_\phi - \hat{\Theta}_\phi, \quad (\text{A4a})$$

$$\hat{\Theta}_{\text{gr}} = -\frac{3\pi G}{4} \left[\sqrt{|\hat{v}|} (\hat{N} - \hat{N}^{-1}) \sqrt{|\hat{v}|} \right]^2, \quad \hat{\Theta}_\phi = \left[\mathbb{I}_{\text{gr}} \otimes \hat{\pi}_\phi^2 + 2\alpha^2 \hat{v}^2 \otimes \tilde{V}(\tilde{\phi}) \right]. \quad (\text{A4b})$$

Taking one of the superselected sectors (e.g. the one corresponding to the positive frequencies), one arrives to the *formal* Schrödinger equation

$$i\partial_\varphi \Psi(v, \phi) = \sqrt{\hat{\Theta}} \Psi(v, \phi). \quad (\text{A5})$$

To write it precisely one needs to overcome several obstacles as $\hat{\Theta}$ is neither positive definite nor essentially self-adjoint [60], since it contains the potential term acting as effective positive cosmological constant on $\phi = \text{const}$ plane. It is however expected to admit a family of non-unique selfadjoint extensions. Therefore one has to choose one extension $\hat{\Theta}_\beta$ (where β is an abstract extension label). Then, upon fixing the gauge $t = \varphi$, the Schroedinger equation can be written as

$$i\partial_t \Psi(v, \phi) = \hat{\mathbf{H}}_\beta \Psi(v, \phi) := \sqrt{[\hat{\Theta}_\beta]_+} \Psi(v, \phi), \quad (\text{A6})$$

where $[\cdot]_+$ denotes the positive part of the operator. Since only the positive part of $\hat{\Theta}_\beta$ enters the Hamiltonian, the physical Hilbert space does not coincide with \mathcal{H}_{kin} . Instead, it is its proper subspace \mathcal{H}_β spanned by the eigenfunctions of $[\hat{\Theta}_\beta]_+$. In principle, different extensions could produce different physical subspaces, as it is the case for positive cosmological constant [51]. The consequence of the latter is that every operator defined on \mathcal{H}_{kin} has to be further projected on \mathcal{H}_β to define the physical operator, thus the operators like \hat{v} lose their simple analytical form.

Proceeding with the construction of the effective description requires a heuristic assumption: namely, that for sufficiently large class of states the projection does not affect the action of the elementary operators significantly. Given that, we can replace \hat{v}^n and \hat{N} by their expectation values, arriving to the Hamiltonian

$$\mathbf{H}_{\text{eff}} = \sqrt{3\pi G v^2 \sin^2(b) - \pi_\phi^2 - 2\alpha^2 v^2 \tilde{V}(\tilde{\phi})} = p_\varphi =: E_\varphi. \quad (\text{A7})$$

Similarly to the dust time case, this (also heuristic) step corresponds to the 0th order effective expansion introduced in [46]. Here, however, this procedure is not fully justifiable, since it ignores the effects of inequivalent self-adjoint extensions on the dynamics (see the discussion in [47]) – effects that, although small, are usually present [51].

If we accept the heuristic steps discussed above, we arrive to an effective model described by the Hamiltonian (A7). To compare it against the treatment of Sec. V we note that:

- (i) For $p_\varphi \neq 0$ the model is equivalent to the one described by the Hamiltonian

$$\mathbf{H}'_{\text{eff}} = 3\pi G v^2 \sin^2(b) - \pi_\phi^2 - 2\alpha^2 v^2 \tilde{V}(\tilde{\phi}). \quad (\text{A8})$$

The equations of motion of this model are equivalent to the one of (A7) with the lapse function rescaled via $N \rightarrow 2p_\varphi N$.

- (ii) Under the change of sign and the lapse function transformation $N \rightarrow N/(2\alpha v)$ the Hamiltonian (A8) transforms into the effective Hamiltonian of the system with dust time (5.2).

⁷ See [28] of the detailed description in the case of vacuum with massless scalar field.

In consequence, at the level of 0th order effective dynamics the deparametrization with respect to massless scalar field and irrotational dust are physically equivalent.

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