Hybrid quantization of an inflationary universe

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We quantize to completion an inflationary universe with small inhomogeneities in the framework of loop quantum cosmology. The homogeneous setting consists of a massive scalar field propagating in a closed, homogeneous scenario. We provide a complete quantum description of the system employing loop quantization techniques. After introducing small inhomogeneities as scalar perturbations, we identify the true physical degrees of freedom by means of a partial gauge fixing, removing all the local degrees of freedom except the matter perturbations. We finally combine a Fock description for the inhomogeneities with the polymeric quantization of the homogeneous background, providing the quantum Hamiltonian constraint of the composed system. Its solutions are then completely characterized, owing to the suitable choice of quantum constraint, and the physical Hilbert space is constructed. Finally, we consider the analog description for an alternate gauge and, moreover, in terms of gauge-invariant quantities. In the deparametrized model, all these descriptions are unitarily equivalent at the quantum level.

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I. INTRODUCTION

Several approaches attempt to combine the current classical description of the gravitational interaction with the principles of the quantum theory. One of the most promising candidates is the so-called Loop Quantum Gravity (LQG) [1], a non-perturbative, background-independent, canonical quantization of General Relativity. Its application to cosmological models is known as Loop Quantum Cosmology (LQC) [2]. All the systems which have been quantized in this framework show the same remarkable property: the classical big-bang singularity is replaced by a quantum bounce. This is indeed the case of massless scalar fields propagating in Friedmann-Robertson-Walker (FRW) scenarios with flat [3], closed [4], or open topologies [5], with cosmological constant [6], or even in spacetimes with anisotropies [7]. Also inhomogeneous systems have been studied, both perturbatively, considering tensor [8], vector [9], and scalar [10, 11] perturbations, and non-perturbatively, as in the case of Gowdy cosmologies in vacuo [12–14] and with matter content [15]. Considerable progress has been reached in situations in which the inhomogeneities propagate as a field in an *effective* background, where quantum corrections in the geometry have been partly incorporated. The analytic and numerical analysis carried out in Ref. [14] (treating the field classically) showed that, even in the presence of non-perturbative inhomogeneities (and disregarding the possibility of extreme fine-tuning conditions), the quantum bounce persists. However, a more fundamental description can be achieved when the field and the background are both treated quantum mechanically, so that, in particular, their interaction is not limited to conform to any particular effective dynamics [16]. This issue has been already addressed in Refs. [12, 13, 15], making use of the fact that Gowdy scenarios with T^3 spatial topology, after a suitable gauge fixing, can be interpreted as a scalar field propagating in a Bianchi I cosmology. A completely quantum description of those models was achieved through a hybrid quantization scheme, proposed initially in Ref. [12], which combines LQC quantization techniques for the homogeneous sector with a standard Fock representation for the inhomogeneous degrees of freedom. In this approach, after a partial gauge fixing, the spatial average of the Halmitonian constraint is imposed quantum mechanically, and the physical Hilbert space is constructed out of its solutions.

Despite the variety of cosmological settings described above, more attention needs to be drawn to inflationary scenarios, given their fundamental role in the physics of the Early Universe [17]. Among all these scenarios, the case of a massive scalar field propagating in an FRW spacetime is of special interest: it is one of the simplest inflationary models keeping most of the required aspects for the satisfactory understanding of our universe. Recently, it has been possible to prove –at the LQC effective dynamics level– that almost all of its solutions provide enough inflation [18], solving the fine-tuning problem arising in General Relativity. However, such promising results do not follow from any genuine quantum dynamics, owing to the lack of a complete quantization of the system. On the other hand, inflationary universes provide a natural framework for the development of primordial cosmological perturbations [19]. The origin of those inhomogeneities could be explained by the assumption that they stem from the early vacuum fluctuations of the inflaton field. Assuming they were initially small, one can invoke perturbation theory to treat them [20, 21]. As far as observations are involved, scalar perturbations are the most interesting ones, since they are those that leave stronger imprints, e.g., in the cosmic microwave background. Thus, they have been observed with high

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precision by the Wilkinson Microwave Anisotropy Probe (WMAP) [22]. Though, even when this type of inhomogeneities has been partially analyzed in LQC inflationary models [10, 11], it is essential to confront the results achieved so far with those that could be obtained from a complete quantization of the perturbed system, without any restriction to a particular effective background.

To approach this problem, in this article we will carry out a complete quantization of an inflationary cosmological model with small inhomogeneities. In a first step, we will consider a homogeneous massive scalar field propagating in a closed FRW scenario [23]. A quantum Hamiltonian constraint is provided and its solutions are characterized. Specifically, it is noted that they are completely determined by their initial data on the minimum volume section allowed by the discretization of the geometry. The physical Hilbert space can be constructed out of this space of initial data just by equipping it with a suitable inner product. Once the homogeneous setting is established, we will introduce small inhomogeneities around the homogeneous solutions by means of perturbation theory. We will carry out a gauge fixing (adopting the longitudinal gauge), and a canonical transformation which includes the scaling of the matter perturbation by the FRW scale factor. The aim of such a transformation is to achieve a formulation of the system in which the dynamical behavior of the matter perturbation approaches, in the ultraviolet limit, the one of a scalar field propagating in a static spacetime with an effective mass owing to the interaction with the FRW background. Next, we will proceed to quantize the system employing a hybrid approach, i.e., we will apply a polymeric quantization to the homogeneous sector while adopting a Fock representation for the inhomogeneities. The problem that then arises concerns the selection of a particular Fock quantization, as we have at our disposal infinite inequivalent representations. Fortunately, the recent uniqueness results for fields in non-stationary spacetimes [25] motivate us to pick up the family of Fock representations in which the vacuum state is invariant under the group of spatial isometries –namely, the $SO(4)$ group– and where the classical dynamics of the field (obtained after deparametrization) is implemented by a unitary quantum operator. It has been possible to prove [26] that this family is indeed a unique unitary equivalence class, as in the situations treated in Ref. [25]. This result is closely tied to the previously mentioned canonical transformation, since a different (non-trivial) scaling of the field prevents the unitary implementation of its corresponding dynamics. Finally, we will formally provide the quantum Hamiltonian constraint of the system and its solutions, and endow them with a Hilbert space structure, thus obtaining the physical Hilbert space.

In order to show the robustness of the treatment and avoid problems related with the choice of a specific gauge, we repeat the procedure for an alternate gauge, in which the spatial metric is homogeneous. Moreover, in both situations we relate the modes of the resulting canonical pair of fields with a set of Bardeen potentials [21], which are gauge invariants of the model, and prove that the canonical transformations relating our fundamental fields with these potentials are unitarily implementable in the quantum theory.

This article is organized as follows. In Sec. II we provide a classical description and the complete quantization of the homogeneous system. The inhomogeneities are included at the classical level in Sec. III, and a complete hybrid quantization of the system is carried out in Sec. IV for a particular gauge choice. In Sec. V, we repeat the same analysis for an alternate gauge fixing. A description in terms of Bardeen potentials can be found in Sec. VI. A summary with the main conclusions is given in Sec. VII. Finally, to make the paper self-contained, four appendixes have been included.

II. THE HOMOGENEOUS AND ISOTROPIC SYSTEM

In this section, we will deal with the homogeneous and isotropic setting, which consists of a massive scalar field propagating in a closed FRW spacetime. We will give a classical description of the corresponding constrained system and proceed to quantize the model to completion, determining the physical Hilbert space. Concerning the technical aspects of the quantization, we will mainly follow Ref. [4].

A. Classical system

The FRW spacetime under consideration can be foliated in spatial sections isomorphic to three-spheres. On them, we choose as fiducial metric the standard round metric of unit radius (instead of radius $a_0 = 2$ as in Ref. [4]), with fiducial volume $l_0^3 = 2\pi^2$.

The degrees of freedom of the matter sector –without taking into account constraints– are a massive scalar field ϕ and its canonically conjugate momentum p_ϕ, while the geometry will be described in terms of an Ashtekar-Barbero connection $A_a^i = c\ {}^0\omega_a^i/l_0$ and a densitized triad $E_i^a = p\sqrt{\Omega}\ {}^0e_i^a/l_0^2$, with i being the internal $SU(2)$ index and a the spatial one, both running from 1 to 3. Here, $\Omega_{ab} = {}^0\omega_a^i\ {}^0\omega_b^i$ is the fiducial metric of the spatial sections, and Ω its determinant. The classical algebra is given by $\{\phi, p_\phi\} = 1$ and $\{c, p\} = 8\pi G\gamma/3$, where G and γ are the Newton constant and the Immirzi parameter, respectively.

Owing to the homogeneity and isotropy, only the Hamiltonian constraint $\mathbb{H} = \bar{N}_0 C_0/(16\pi G)$ remains, where $\bar{N}_0$ is the (homogeneous) lapse function,

$$C_0 = -\frac{6\sqrt{|p|}}{\gamma^2}[(c-l_0)^2 + \gamma^2 l_0^2] + \frac{8\pi G}{V}\left(p_\phi^2 + m^2V^2\phi^2\right), \tag{2.1}$$

and $V = |p|^{3/2}$.

B. Quantum system

In the quantization of the system, we choose a standard Schrödinger representation for the scalar field, whose kinematical Hilbert space is $\mathcal{H}_{\rm kin}^{\rm mat} = L^2(\mathbb{R}, d\phi)$. For the geometry, we apply a polymeric quantization [2]. The basic variables in LQC are fluxes of densitized triads through square surfaces, enclosed by four geodesic edges, which are basically given by p, and holonomies of the connection along integral curves of the fiducial triads of fiducial length μl_0. The gravitational part of the kinematical Hilbert space is $\mathcal{H}_{\rm kin}^{\rm grav} = L^2(\mathbb{R}_{\rm Bohr}, d\mu_{\rm Bohr})$, where $\mathbb{R}_{\rm Bohr}$ is the Bohr compactification of the real line, and $d\mu_{\rm Bohr}$ is the natural Haar measure associated with it. Then, the kinematical Hilbert space of the whole system is the tensor product $\mathcal{H}_{\rm kin}^{\rm mat} \otimes \mathcal{H}_{\rm kin}^{\rm grav}$.

To promote the Hamiltonian constraint to a quantum operator, its gravitational part must be written in terms of holonomies of the connection A_a^i. We will essentially follow the procedure of Ref. [4], where the curvature tensor constructed out of $su(2)$-connections is regularized. As a first step, one constructs holonomies along the edges of a closed square, properly selected by considering four integral curves along alternating left and right invariant vector fields (left and right invariant vector fields commute), well adapted to the fiducial structures. Then, the curvature operator is basically replaced by a circuit of holonomies around a square enclosing a non-vanishing area Δ, determined by the infrared spectrum of the area operator defined in LQG (classically, the local curvature would be recovered in the limit $\Delta \to 0$). As in Ref. [4], we adhere to the *improved dynamics* scheme, in which the fiducial length of the edges of the considered square is given by the function $\bar{\mu} = \sqrt{\Delta/p}$, up to a factor l_0. In the triad representation, one can find a basis of normalizable states $|v\rangle$ in $\mathcal{H}_{\rm kin}^{\rm grav}$ (with $v \in \mathbb{R}$), on which the action of the matrix elements of the holonomies is $\hat{N}_{\bar{\mu}}|v\rangle = |v+1\rangle$, while $\hat{p}|v\rangle = {\rm sgn}(v)(2\pi\gamma G\hbar\sqrt{\Delta}|v|)^{2/3}|v\rangle$, with $\hbar$ being the Planck constant.

Finally, we adopt the following operator as quantum Hamiltonian constraint:

$$\hat{C}_0 = \widehat{\left[\frac{1}{V}\right]}^{1/2} \Bigg[8\pi G\big(\hat{p}_\phi^2 + m^2\hat{V}^2\hat{\phi}^2\big) - \frac{6}{\gamma^2}\widehat{\Omega}^2 - \frac{6}{\gamma^2}\left\{(1+\gamma^2)l_0^2\hat{V}^{4/3} - \frac{\hat{V}^2}{\Delta}\sin^2(\hat{\bar{\mu}}l_0)\right\}\Bigg] \widehat{\left[\frac{1}{V}\right]}^{1/2}, \tag{2.2}$$

where $\hat{V}$ represents the volume $V = |p|^{3/2}$, and we have introduced the inverse of this operator, defined as

$$\widehat{\left[\frac{1}{V}\right]} = \widehat{{\rm sgn}(v)}\hat{V}\left[\frac{3}{4\pi\gamma G\hbar\sqrt{\Delta}}(\hat{N}_{-\bar{\mu}}\hat{V}^{1/3}\hat{N}_{\bar{\mu}} - \hat{N}_{\bar{\mu}}\hat{V}^{1/3}\hat{N}_{-\bar{\mu}})\right]^3. \tag{2.3}$$

In addition,

$$\widehat{\Omega} = \frac{1}{4i\sqrt{\Delta}}\hat{V}^{1/2} \times \Big[\widehat{{\rm sgn}(v)}\left(e^{-i\frac{\hat{\bar{\mu}}l_0}{2}}\hat{N}_{2\bar{\mu}}e^{-i\frac{\hat{\bar{\mu}}l_0}{2}} - e^{i\frac{\hat{\bar{\mu}}l_0}{2}}\hat{N}_{-2\bar{\mu}}e^{i\frac{\hat{\bar{\mu}}l_0}{2}}\right) + \left(e^{-i\frac{\hat{\bar{\mu}}l_0}{2}}\hat{N}_{2\bar{\mu}}e^{-i\frac{\hat{\bar{\mu}}l_0}{2}} - e^{i\frac{\hat{\bar{\mu}}l_0}{2}}\hat{N}_{-2\bar{\mu}}e^{i\frac{\hat{\bar{\mu}}l_0}{2}}\right)\widehat{{\rm sgn}(v)}\Big]\hat{V}^{1/2}. \tag{2.4}$$

The constraint $\hat{C}_0$ annihilates the state $|v = 0\rangle$ and leaves invariant its orthogonal complement. Therefore, we can decouple the state corresponding to the classical singularity, i.e., $|v = 0\rangle$, and restrict the study to its orthogonal complement, that will be denoted from now on by $\widetilde{\mathcal{H}}_{\rm kin}^{\rm grav}$. Besides, with the usual definition of $\sin(\hat{\bar{\mu}}l_0)$ (see Ref. [4]), $\widehat{\Omega}^2$ is the only operator in the constraint with a non-diagonal action on the v-basis of $\widetilde{\mathcal{H}}_{\rm kin}^{\rm grav}$. It only relates states with support on isolated points separated by a constant step of 4 units in the label v and, moreover, different orientations of the triad are decoupled. In conclusion, only states with support on semilattices $\mathcal{L}_\varepsilon^\pm = \{v = \pm(\varepsilon + 4n);\, n \in \mathbb{N}\}$ are related by the action of $\widehat{\Omega}^2$, where $\varepsilon \in (0, 4]$ is a continuous parameter proportional to the minimum value of the physical volume of the system in the sector under consideration. Let us emphasize that those sectors are preserved by all the operators of physical interest considered in this article. Consequently, they can be interpreted as superselection sectors, denoted from now on as $\mathcal{H}_\pm^\varepsilon$.

In the following, and without loss of generality, we will restrict our study to $\mathcal{H}_+^\varepsilon$. Besides, we will apply a unitary transformation $\hat{U} = e^{il_0\hat{h}(v)}$ on $\mathcal{H}_+^\varepsilon$, where $h(v)$ is defined in Appendix A, in complete parallelism with the analyses carried out in Ref. [4]. This unitary transformation maps $\widehat{\Omega}^2$ into

$$\widehat{\Omega}_0^2 = \hat{U}\widehat{\Omega}^2\hat{U}^{-1}, \tag{2.5}$$

which is equivalent to the analog operator for a scenario with flat topology

$$\widehat{\Omega}_0 = \frac{1}{4i\sqrt{\Delta}}\hat{V}^{1/2}\Big[\widehat{{\rm sgn}(v)}\big(\hat{N}_{2\bar{\mu}} - \hat{N}_{-2\bar{\mu}}\big) + \big(\hat{N}_{2\bar{\mu}} - \hat{N}_{-2\bar{\mu}}\big)\widehat{{\rm sgn}(v)}\Big]\hat{V}^{1/2}, \tag{2.6}$$

just like the operator suggested in Ref. [27], but without inverse volume corrections (see Ref. [28] for additional information).

Hence, the gravitational part of the quantum Hamiltonian constraint is finally encoded by

$$\hat{C}_{\rm grav} = \widehat{\left[\frac{1}{V}\right]}^{1/2}\hat{\mathcal{C}}_{\rm grav}\widehat{\left[\frac{1}{V}\right]}^{1/2}, \tag{2.7}$$

with

$$\hat{\mathcal{C}}_{\rm grav} = -\frac{6}{\gamma^2}\left\{\widehat{\Omega}_0^2 - \frac{\hat{V}^2}{\Delta}\sin^2(\hat{\bar{\mu}}l_0) + (1+\gamma^2)l_0^2\hat{V}^{4/3}\right\}. \tag{2.8}$$

As an aside, let us comment that, following the arguments of Ref. [4] (applied there to a related operator, $\hat{\Theta}$), and noticing that the superselection sectors are now semilattices (instead of full lattices as in that work), it seems reasonable to admit that the restriction of $\hat{\mathcal{C}}_{\rm grav}$ to $\mathcal{H}_+^\varepsilon$ provides a self-adjoint operator with a non-degenerate discrete spectrum.

The solutions $(\Psi|$ annihilated by the constraint $\hat{C}_0$ can be defined in the dual of a dense set in $\mathcal{H}_{\rm kin}^{\rm mat}\otimes\mathcal{H}_+^\varepsilon$, e.g., that of the product of the span of the v-basis and the functions of ϕ with compact support. It is straightforward to see that the coefficients $\Psi(v,\phi)=(\Psi|v,\phi\rangle$ satisfy a difference equation that resembles an evolution equation with v playing the role of an internal time. Besides, one can check that the initial data $\Psi(\varepsilon,\phi)$ determines the whole solution at any volume $v=\varepsilon+4n$, $\forall n\in\mathbb{N}$, in the considered semilattice. Therefore, we can identify these initial data with the solutions, and complete the space of such data with an adequate inner product in order to reach the physical Hilbert space [29]. In this way, the physical Hilbert space can be taken as $\mathcal{H}^{\rm phys}=L^2(\mathbb{R},d\phi)$.

III. INHOMOGENEITIES: CLASSICAL DESCRIPTION

In this section we will introduce small inhomogeneities in the model, treating them as perturbations. Specifically, we will expand the Hamiltonian constraint up to second order in those perturbations. We will follow the same classical approach as in Ref. [31]. Besides, we will carry out a gauge fixing in order to remove the unphysical degrees of freedom. Finally, we will introduce a suitable canonical transformation to prepare the system for its hybrid quantization, performed in Sec. IV.

A. Perturbations around classical homogeneous solutions.

We now briefly revisit the inclusion of inhomogeneities in our cosmological model as perturbations of the homogeneous system. For convenience, we introduce a perturbative parameter ϵ, making proportional to it each of the inhomogeneous corrections to the geometry and the matter field. Using this parameter, we carry out a perturbative expansion in the action, expressed in Hamiltonian form, and truncate the expansion at second order. Furthermore, for simplicity, we will only consider scalar perturbations, something which is consistent at the studied perturbative order because they are decoupled from genuine vector and tensor perturbations of the system in this approximation [31]. Our focus on scalar perturbations is mainly motivated by their relevant role in observational cosmology. In addition, we adopt a natural expansion of the inhomogeneities in terms of modes of the Laplace-Beltrami operator in the three-sphere, namely, the (hyper-)spherical harmonics in S^3: Q^n, P_a^n, and P_{ab}^n (see Appendix B), where we recall that Latin indices from the beginning of the alphabet denote spatial indices, and $n\in\mathbb{N}^+$ is here [32] a positive integer that labels the eigenvalues of the Laplace-Beltrami operator [see Eq. (B1)]. Let us then write

$$N=\sigma N_0\Big(1+\sqrt{2}\pi\epsilon\sum_n g_nQ^n\Big), \tag{3.1}$$

$$N_a=\sigma^2e^{\alpha}\sqrt{2}\pi\epsilon\sum_n k_nP_a^n, \tag{3.2}$$

$$h_{ab}=\sigma^2e^{2\alpha}\Big[\Omega_{ab}+2^{3/2}\pi\epsilon\sum_n(a_nQ^n\Omega_{ab}+3b_nP_{ab}^n)\Big], \tag{3.3}$$

$$\Phi=\frac{1}{\sigma}\Big[\frac{\varphi}{\sqrt{2}\pi}+\epsilon\sum_n f_nQ^n\Big]. \tag{3.4}$$

In these formulas, $\sigma^2=4\pi G/(3l_0^3)$, and the unperturbed scalar field has mass $m=\tilde{m}/\sigma$. In order to facilitate comparison with the analysis of Ref. [31], as well as to apply the results of Ref. [26], we employ here the variables α, φ, and their corresponding momenta π_α and π_φ, to describe the homogeneous sector. In the absence of inhomogeneities (i.e., in the unperturbed system), the relation with the homogeneous variables used in Sec. II A is given by

$$|p|=l_0^2\sigma^2e^{2\alpha},\qquad p(c-l_0)=-\gamma l_0^3\sigma^2\pi_\alpha, \tag{3.5}$$

$$\phi=\frac{\varphi}{l_0^{3/2}\sigma},\qquad p_\phi=l_0^{3/2}\sigma\pi_\varphi. \tag{3.6}$$

Note that the correspondence between $\alpha\in\mathbb{R}$ and the flux variable p is one-to-one, e.g., in the union of all the superselection sectors $\mathcal{H}_+^\varepsilon$, to which we are particularizing our discussion.

For the inhomogeneities, on the other hand, the canonically conjugate momenta of the coefficients a_n, b_n, and f_n will be denoted by π_{a_n}, π_{b_n}, and π_{f_n}, respectively, while g_n and k_n play the role of Lagrange multipliers associated with two linear constraints.

Truncating the action at quadratic order in ϵ, we obtain the total Hamiltonian:

$$\mathbb{H}=N_0\Big[H_0+\epsilon^2\sum_n\big(H_2^n+g_nH_{|1}^n\big)\Big]+\epsilon^2\sum_n k_nH_{\_1}^n, \tag{3.7}$$

where H_0 corresponds to the Hamiltonian constraint of the homogeneous sector,

$$H_0=\frac{e^{-3\alpha}}{2}(-\pi_\alpha^2+\pi_\varphi^2+e^{6\alpha}\tilde{m}^2\varphi^2-e^{4\alpha}), \tag{3.8}$$

and for each mode n we have

$$
\begin{aligned}
H_2^n = \frac{e^{-3\alpha}}{2}\Bigg[&\left(\frac{1}{2}a_n^2 + 10\frac{n^2-4}{n^2-1}b_n^2\right)\pi_\alpha^2 + \left(\frac{15}{2}a_n^2 + 6\frac{n^2-4}{n^2-1}b_n^2\right)\pi_\varphi^2 - \pi_{a_n}^2 + \frac{n^2-1}{n^2-4}\pi_{b_n}^2 + \pi_{f_n}^2 - 6a_n\pi_{f_n}\pi_\varphi \\
&+ \big(2a_n\pi_{a_n} + 8b_n\pi_{b_n}\big)\pi_\alpha - e^{4\alpha}\left\{\frac{1}{3}\big(n^2 - \tfrac{5}{2}\big)a_n^2 + \frac{1}{3}\big(n^2-7\big)\frac{n^2-4}{n^2-1}b_n^2 + \frac{2}{3}\big(n^2-4\big)a_n b_n - \big(n^2-1\big)f_n^2\right\} \\
&+ e^{6\alpha}\tilde{m}^2\left(\frac{3}{2}\varphi^2 a_n^2 - 6\frac{n^2-4}{n^2-1}\varphi^2 b_n^2 + f_n^2 + 6\varphi a_n f_n\right)\Bigg], \qquad (3.9)
\end{aligned}
$$

$$
H_{|1}^n = \frac{e^{-3\alpha}}{2}\left[2(\pi_\varphi\pi_{f_n} - \pi_\alpha\pi_{a_n}) - (\pi_\alpha^2 + 3\pi_\varphi^2)a_n - \frac{2}{3}e^{4\alpha}\left\{\big(n^2+\tfrac{1}{2}\big)a_n + \big(n^2-4\big)b_n\right\} + e^{6\alpha}\tilde{m}^2\varphi\big(2f_n + 3\varphi a_n\big)\right], \qquad (3.10)
$$

$$
H_{\_1}^n = \frac{e^{-\alpha}}{3}\left[\left(a_n + 4\frac{n^2-4}{n^2-1}b_n\right)\pi_\alpha - \pi_{a_n} + \pi_{b_n} + 3f_n\pi_\varphi\right]. \qquad (3.11)
$$

Here, H_2^n and $H_{|1}^n$ are the scalar constraints quadratic and linear in the perturbations, respectively, and $H_{\_1}^n$ is the diffeomorphism constraint, also linear in the inhomogeneities. Finally, note that, substituting $\bar{N}_0 = \sigma N_0$, the homogeneous constraint (2.1) reproduces $16\pi G H_0$ as given in Eq. (3.8), under the changes (3.5) and (3.6).

B. Gauge fixing

For each mode $n = 3, 4, 5, ...$, there are three dynamical degrees of freedom in the inhomogeneous sector: a_n, b_n, and f_n, and two linear constraints: $H_{|1}^n$ and $H_{\_1}^n$. The modes $n = 1$ and $n = 2$, on the other hand, will be treated independently, since they are in fact pure gauge. Hence, for $n \geq 3$, two non-physical degrees of freedom can be removed by means of a gauge fixing. Let us consider the longitudinal gauge, which is fixed by imposing the conditions

$$
b_n = 0, \quad \Pi_n = \pi_{a_n} - \pi_\alpha a_n - 3\pi_\varphi f_n = 0. \qquad (3.12)
$$

These conditions provide an admissible gauge since they are second class with the linear momentum and Hamiltonian constraints. Besides, we can find values of k_n and g_n for which these gauge-fixing conditions are stable in the evolution. A simple computation yields that, on the gauge-fixed section,

$$
\{b_n, \mathbb{H}\} = 0 \Leftrightarrow k_n = -3\frac{n^2-1}{n^2-4}N_0 e^{-2\alpha}\pi_{b_n}, \qquad (3.13)
$$

$$
\{\Pi_n, \mathbb{H}\} = 0 \Leftrightarrow g_n = -a_n. \qquad (3.14)
$$

Finally, if the conditions $H_{|1}^n = H_{\_1}^n = 0$ are satisfied, we can eliminate π_{b_n}, a_n, and π_{a_n} in favor of f_n and π_{f_n}. At this point we want to emphasize that, unlike the vanishing modes (b_n, π_{b_n}), neither a_n nor π_{a_n} is equal to zero. Therefore, the reduced symplectic structure in the gauge-fixed system has a canonical form only in a suitable new set of variables on the reduced phase space.

Let us introduce the following set:

$$
\tilde{\alpha} = \alpha + \epsilon^2\sum_n \frac{a_n^2}{2}, \qquad (3.15)
$$

$$
\tilde{\varphi} = \varphi + \epsilon^2\sum_n 3a_n f_n, \qquad (3.16)
$$

$$
\tilde{\pi}_\alpha = \pi_\alpha, \quad \tilde{\pi}_\varphi = \pi_\varphi, \qquad (3.17)
$$

$$
\tilde{f}_n = f_n, \quad \tilde{\pi}_{f_n} = \pi_{f_n} - 3a_n\pi_\varphi, \qquad (3.18)
$$

where, after reduction, it is understood that

$$
\pi_{a_n} = a_n\tilde{\pi}_\alpha + 3f_n\tilde{\pi}_\varphi, \qquad (3.19)
$$

$$
a_n = 3\frac{\tilde{\pi}_\varphi\tilde{\pi}_{f_n} + (e^{6\tilde{\alpha}}\tilde{m}^2\tilde{\varphi} - 3\tilde{\pi}_\alpha\tilde{\pi}_\varphi)\tilde{f}_n}{e^{4\tilde{\alpha}}(n^2-4)}, \qquad (3.20)
$$

at the considered perturbative order. For simplicity in the notation, we have used a_n in most of the expressions above, but one must keep in mind that its value is given by Eq. (3.20).

The reduced Hamiltonian constraint in this new set of variables, truncated to the correct perturbative order, is

$$
\tilde{\mathbb{H}} = N_0\Big(\tilde{H}_0 + \epsilon^2\sum_n \tilde{H}_2^n\Big), \qquad (3.21)
$$

where $\tilde{H}_0$ has formally the same expression as H_0, but now in terms of the new variables $\tilde{\alpha}$, $\tilde{\varphi}$, $\tilde{\pi}_\alpha$, and $\tilde{\pi}_\varphi$ [see Eq. (3.8)], and

$$
\begin{aligned}
\tilde{H}_2^n &= \frac{e^{-3\tilde{\alpha}}}{2}\Big(\tilde{\pi}_{f_n}^2\tilde{E}_{\pi\pi}^n + \tilde{f}_n\tilde{\pi}_{f_n}\tilde{E}_{f\pi}^n + \tilde{f}_n^2\tilde{E}_{ff}^n\Big), \\
\tilde{E}_{\pi\pi}^n &= 1 - \frac{3\tilde{\pi}_\varphi^2}{e^{4\tilde{\alpha}}(n^2-4)}, \\
\tilde{E}_{f\pi}^n &= 6\tilde{\pi}_\varphi\frac{3\tilde{\pi}_\alpha\tilde{\pi}_\varphi - e^{6\tilde{\alpha}}\tilde{m}^2\tilde{\varphi}}{e^{4\tilde{\alpha}}(n^2-4)}, \\
\tilde{E}_{ff}^n &= e^{4\tilde{\alpha}}(n^2-1) + e^{6\tilde{\alpha}}\tilde{m}^2 - 9\tilde{\pi}_\varphi^2 \\
&\quad - 3\frac{(e^{6\tilde{\alpha}}\tilde{m}^2\tilde{\varphi} - 3\tilde{\pi}_\alpha\tilde{\pi}_\varphi)^2}{e^{4\tilde{\alpha}}(n^2-4)}.
\end{aligned} \qquad (3.22)
$$

Finally, we deal with the modes $n = 1$ and 2. For each of these cases, we only have two configuration variables, a_n and f_n, and their corresponding momenta. Owing to the presence of the diffeomorphism constraint and the linear scalar constraint, these modes are completely constrained. A convenient gauge fixing for them is $a_n = f_n = 0$. Then, the constraints $H^n_{|1} = H^n_{\_1} = 0$ imply that their corresponding momenta vanish. These conditions are stable under the dynamics if $g_n = k_n = 0$.

C. Canonical transformation

Now that the system has been reduced, we will change variables on the canonical phase space to adapt it to the requirements of the uniqueness results provided in Refs. [25, 26], regarding the quantization of fields in non-stationary scenarios after deparametrization. Specifically, any $SO(4)$-invariant Fock representation that implements the dynamics unitarily is only compatible with a particular choice of variables on the phase space of the field, as any genuinely time-dependent linear canonical transformation of those variables prevents the simultaneous fulfillment of both properties in another representation [33]. We can introduce that preferred set of variables by means of a canonical transformation on the reduced phase space. Let us start with: i) a scaling of the field of modes $\tilde{f}_n$ by the FRW scale factor, and ii) the inverse scaling of its momentum, also allowing a suitable momentum shift proportional to the configuration variable. These modifications can be extended straightforwardly to a canonical transformation which involves both the homogeneous and the inhomogeneous sectors. In this way, we arrive at the following variables, which are canonical at the considered perturbative order:

$$\bar{\alpha} = \tilde{\alpha} + \frac{\epsilon^2}{2}\sum_n \tilde{f}_n^2, \quad \bar{\varphi} = \tilde{\varphi}, \quad \bar{\pi}_\varphi = \tilde{\pi}_\varphi,$$
$$\bar{\pi}_\alpha = \tilde{\pi}_\alpha + \epsilon^2 \sum_n \left(\tilde{\pi}_\alpha \tilde{f}_n^2 - \tilde{f}_n \tilde{\pi}_{f_n}\right),$$
$$\bar{f}_n = e^{\tilde{\alpha}}\tilde{f}_n, \quad \bar{\pi}_{f_n} = e^{-\tilde{\alpha}}(\tilde{\pi}_{f_n} - \tilde{\pi}_\alpha \tilde{f}_n). \tag{3.23}$$

After the change, the homogeneous part of the Hamiltonian constraint remains formally the same, though with the old homogeneous variables replaced with the new ones, while the perturbed Hamiltonian at order ϵ^2 is

$$\bar{H}_2^n = \frac{e^{-\bar{\alpha}}}{2}\left(\bar{\pi}_{f_n}^2 \bar{E}^n_{\pi\pi} + \bar{f}_n \bar{\pi}_{f_n} \bar{E}^n_{f\pi} + \bar{f}_n^2 \bar{E}^n_{ff}\right), \tag{3.24}$$

$$\bar{E}^n_{\pi\pi} = 1 - \frac{3\bar{\pi}_\varphi^2}{e^{4\bar{\alpha}}(n^2-4)},$$
$$\bar{E}^n_{f\pi} = 6\bar{\pi}_\varphi \frac{2\bar{\pi}_\alpha\bar{\pi}_\varphi - e^{6\bar{\alpha}}\tilde{m}^2\bar{\varphi}}{e^{6\bar{\alpha}}(n^2-4)},$$
$$\bar{E}^n_{ff} = n^2 - 1 - \frac{\bar{\pi}_\alpha^2 + 15\bar{\pi}_\varphi^2 - e^{4\bar{\alpha}} + 3e^{6\bar{\alpha}}\tilde{m}^2\bar{\varphi}^2}{2e^{4\bar{\alpha}}} + e^{2\bar{\alpha}}\tilde{m}^2 - 3\frac{(2\bar{\pi}_\alpha\bar{\pi}_\varphi - e^{6\bar{\alpha}}\tilde{m}^2\bar{\varphi})^2}{e^{8\bar{\alpha}}(n^2-4)}. \tag{3.25}$$

This description of the reduced phase space, and of its Hamiltonian constraint, will be our starting point for the hybrid approach, except for a convenient transformation in the homogeneous sector of the phase space, carried out to reintroduce a natural set of variables for its polymeric quantization. This transformation leads from $\bar{\alpha}$, $\bar{\pi}_\alpha$, $\bar{\varphi}$, and $\bar{\pi}_\varphi$ to variables that are formally similar to p, c, ϕ, and p_ϕ, namely the variables introduced in Sec. II A, though defined now in coexistence with the inhomogeneities. The change is given again by Eqs. (3.5) and (3.6), replacing the old variables with their barred counterpart. Besides, we will call C_0 and C_2^n, respectively, the constraints $\bar{H}_0$ and $\bar{H}_2^n$ expressed in terms of these new variables for the homogeneous sector, and multiplied by a factor of $16\pi G = 12 l_0^3 \sigma^2$ in order to adopt the usual conventions employed in LQC.

IV. HYBRID QUANTIZATION

As we have anticipated, our main aim is to accomplish a complete quantization of this inflationary model containing inhomogeneities. As a preliminary step, we will introduce an auxiliary quantum framework –the so-called kinematical Hilbert space– to construct a quantum representation of the classical system, and in particular, of the Hamiltonian constraint. In order to determine the physical sector, we will look for the states annihilated by this quantum constraint, and build the physical Hilbert space out of them.

A. Kinematical Hilbert space

Let us consider again the kinematical Hilbert space $\mathcal{H}^{\text{mat}}_{\text{kin}} \otimes \mathcal{H}^{\text{grav}}_{\text{kin}}$ for the homogeneous sector, as explained in Sec. II B. We recall that, in $\mathcal{H}^{\text{mat}}_{\text{kin}}$, the operator $\hat{\phi}$ acts by multiplication and its conjugate variable $\hat{p}_\phi$ is a derivative operator. In the gravitational sector, the fundamental variables are fluxes and holonomies of $su(2)$-connections, essentially represented, respectively, by the multiplicative operator $\hat{p}$ and the matrix elements of the holonomies, i.e., $\hat{N}_{\bar{\mu}}$ (in the improved dynamics scheme). Both operators have a well defined action on $\mathcal{H}^{\text{grav}}_{\text{kin}}$.

For the perturbations, in Sec. III C we arrived at a privileged description, given by the variables $\bar{f}_n$ and $\bar{\pi}_{f_n}$, defined in Eq. (3.23). In this description, the massless representation permits a unitary quantum implementation of the field dynamics [26]. To perform a standard Fock quantization, it is hence convenient to rewrite these modes in terms of the corresponding annihilation and creation-like variables, namely a_{f_n} and their complex conjugate $a^*_{f_n}$, with

$$a_{f_n} = \frac{1}{\sqrt{2\omega_n}}(\omega_n \bar{f}_n + i\bar{\pi}_{f_n}), \tag{4.1}$$

and $\omega_n^2 = n^2 - 1$. We promote these variables to quantum operators $\hat{a}_{f_n}$ and $\hat{a}^\dagger_{f_n}$, such that $[\hat{a}_{f_n}, \hat{a}^\dagger_{f_{n'}}] = \delta_{nn'}$. Let us now call $\mathcal{S}$ the vector space consisting of finite linear combinations of the N-particle states

$$|\mathcal{N}\rangle = |N_3, N_4, ...\rangle, \quad \sum_{n\geq 3} N_n < \infty, \tag{4.2}$$

with $N_n \in \mathbb{N}$ being the number of particles of the n-th mode. Then, we can construct the inhomogeneous sector of the kinematical Hilbert space, $\mathcal{F}$, as the completion of $\mathcal{S}$ with respect to the inner product $\langle \mathcal{N}|\mathcal{N}'\rangle = \delta_{\mathcal{N}\mathcal{N}'}$. Obviously, the N-particle states are then an orthonormal basis of the Fock space $\mathcal{F}$. The total kinematical Hilbert space can thus be taken as

$$\mathcal{H}^{\rm kin} = \mathcal{H}^{\rm kin}_{\rm grav} \otimes \mathcal{H}^{\rm kin}_{\rm mat} \otimes \mathcal{F}. \tag{4.3}$$

On this Hilbert space, it is understood that both $\hat{a}_{f_n}$ and $\hat{a}^\dagger_{f_n}$ act as the identity on the homogeneous sector.

B. Quantum constraint

Let us now concentrate our discussion on the Hamiltonian constraint (3.24) after rewriting it in terms of the variables p, c, ϕ, and p_ϕ, as we have commented above. To introduce a(n at least symmetric) operator that represents this constraint on $\mathcal{H}^{\rm kin}$, we admit the natural assumption that the superselection sectors of the homogeneous system (i.e., the sectors $\mathcal{H}^\varepsilon_+$, if we are already restricting the analysis to positive p) are preserved by the inclusion of the inhomogeneities, since the latter are regarded as perturbations of the homogeneous setting. We then adopt the following quantization prescriptions:

1. Contributions like ϕp_ϕ will be promoted to the operator $(\hat{\phi}\hat{p}_\phi + \hat{p}_\phi\hat{\phi})/2$.

2. In any product of a power of the volume V and a non-commuting expression, the former will be evenly distributed around the latter so as to obtain a symmetric combination.

3. Any even power of the form $[(c-l_0)p]^{2k}$, with $k \in \mathbb{Z}$, will be represented by $\widehat{\Theta}^e_{(k)} = [\widehat{\Omega}^2]^k$, constructed using the positive operator $\widehat{\Omega}^2$ [see Eq. (2.4)] and the spectral theorem to define its k-th power [34, 35].

4. In the case of odd powers of the form $[(c-l_0)p]^{2k+1}$, the prescription will be

$$[(c-l_0)p]^{2k+1} \to \widehat{\Theta}^o_{(k)} = |\widehat{\Omega}|^k \widehat{\Lambda} |\widehat{\Omega}|^k, \tag{4.4}$$

where $|\widehat{\Omega}| = \sqrt{\widehat{\Omega}^2}$ and

$$\widehat{\Lambda} = \frac{\hat{V}^{1/2}}{8i\sqrt{\Delta}}\Big[\widehat{\mathrm{sgn}(v)} \sum_{r=+1,-1}\Big(re^{-ir\hat{\bar{\mu}}l_0}\hat{N}_{4r\bar{\mu}}e^{-ir\hat{\bar{\mu}}l_0}\Big) + \sum_{r=+1,-1}\Big(re^{-ir\hat{\bar{\mu}}l_0}\hat{N}_{4r\bar{\mu}}e^{-ir\hat{\bar{\mu}}l_0}\Big)\widehat{\mathrm{sgn}(v)}\Big]\hat{V}^{1/2}. \tag{4.5}$$

One can straightforwardly see that $\widehat{\Lambda}$ is a difference operator which only relates states with support in semilattices of step 4 for v. Therefore, any power of $(c-l_0)p$ will be promoted indeed to an operator that preserves the superselection sectors in this homogeneous volume (see Sec. II B).

Using these assignments, we arrive at a quantum constraint of the form

$$\hat{C} = \hat{C}_0 + \epsilon^2 \sum_n \hat{C}^n_2, \tag{4.6}$$

where $\hat{C}_0$ is the homogeneous constraint defined in Eq. (2.2), and

$$\hat{C}^n_2 = 6l_0^4\sigma^2 \widehat{\left[\frac{1}{V}\right]}^{1/6}\Bigg[\hat{N}^n\Big(2\omega_n + \frac{1}{\omega_n}\hat{F}^n_-\Big) + \frac{1}{2\omega_n}\Big(\hat{X}^n_+\hat{F}^n_+ + \frac{3i\omega_n\sigma^2}{\omega_n^2-3}\hat{X}^n_-\hat{G}\Big)\Bigg]\widehat{\left[\frac{1}{V}\right]}^{1/6}. \tag{4.7}$$

Here

$$\hat{N}^n = \hat{a}^\dagger_{f_n}\hat{a}_{f_n}, \quad \hat{X}^n_\pm = (\hat{a}^\dagger_{f_n})^2 \pm \hat{a}^2_{f_n}, \tag{4.8}$$

$$\hat{F}^n_\pm = -\frac{\sigma^2 l_0}{2}\widehat{\left[\frac{1}{V}\right]}^{2/3}\Bigg(15\hat{p}^2_\phi + 3m^2\hat{V}^2\hat{\phi}^2 + \frac{\widehat{\Theta}^e_{(1)}}{\gamma^2 l_0^3\sigma^2}\Bigg)\widehat{\left[\frac{1}{V}\right]}^{2/3} - \frac{3}{n^2-4}\frac{\sigma^2}{l_0}\widehat{\left[\frac{1}{V}\right]}^{4/3}\Big(\frac{2}{\gamma}\hat{p}_\phi\widehat{\Theta}^o_{(0)} + m^2\hat{V}^2\hat{\phi}\Big)^2\widehat{\left[\frac{1}{V}\right]}^{4/3} + \frac{1}{2} + \frac{m^2}{l_0^2}\hat{p} \pm 3\sigma^2 l_0\frac{n^2-1}{n^2-4}\hat{p}^2_\phi\widehat{\left[\frac{1}{V}\right]}^{4/3}, \tag{4.9}$$

$$\hat{G} = -\widehat{\left[\frac{1}{V}\right]}\Big[m^2\hat{p}^3(\hat{\phi}\hat{p}_\phi + \hat{p}_\phi\hat{\phi}) + \frac{4}{\gamma}\hat{p}^2_\phi\widehat{\Theta}^o_{(0)}\Big]\widehat{\left[\frac{1}{V}\right]}. \tag{4.10}$$

At this stage, it is worth noticing that any possible factor ordering ambiguity affecting $\hat{C}^n_2$, resulting from prescriptions other than ours for its operator representation, produces only subleading quantum geometry corrections to the (already) perturbative terms in the total constraint.

As in the absence of inhomogeneities, the constraint $\hat{C}$ annihilates the state $|v=0\rangle$ (times any state in $\mathcal{H}^{\rm kin}_{\rm mat}\otimes\mathcal{F}$), and leaves invariant its orthogonal complement, $\widetilde{\mathcal{H}}^{\rm kin}$, complement to which we can hence restrict all considerations in the following, removing the state analog of the cosmological (homogeneous) singularity. Besides, as anticipated, the operator $\hat{C}$ preserves the sectors of superselection in the homogeneous volume, namely the (positive) semilattices of step 4 in the label v, since all the basic operators from which $\hat{C}$ is constructed preserve those sectors in fact. In other words, as in the analysis of the homogeneous system, the action on v of all the operators considered in this article preserve the subspaces $\mathcal{H}^\varepsilon_+$ of states with support in the semilattices $\mathcal{L}^+_\varepsilon$ (limiting again the discussion to positive values of v for simplicity).

C. Physical Hilbert space

In order to complete our quantization, we still have to characterize the space of solutions to the constraint $\hat{C}$ and provide it with the structure of a Hilbert space. In accordance with our perturbative approach, we will assume that the solutions can be expanded in a perturbative series and truncate them in the form

$$(\psi| = (\psi|^{(0)} + \epsilon^2 (\psi|^{(2)}. \tag{4.11}$$

In turn, each term can be expanded employing the basis that we have introduced for the total kinematical Hilbert space of the system:

$$(\psi|^{(k)} = \sum_{\mathcal{N}} \sum_{v\in\mathcal{L}_\varepsilon} \int d\phi \langle\mathcal{N}| \otimes \langle v| \otimes \langle\phi|\psi^{(k)}(\mathcal{N}, v, \phi). \tag{4.12}$$

By consistency, the Hamiltonian constraint $(\psi|\hat{C}^\dagger$ must vanish order by order, up to the level of our approximation in the perturbative expansion. Here, the dagger denotes again the adjoint. The zeroth-order contribution to the constraint yields $(\psi|^{(0)}\hat{C}_0^\dagger = 0$. But this condition is just the constraint studied in Sec. II B for the homogeneous sector. Recall that we have shown that the corresponding solutions are completely characterized by the initial data on the minimum volume section $v = \varepsilon$. In addition, note that, at this zeroth order, the information that $(\psi|^{(0)}$ codifies about the inhomogeneities does not change in the evolution in v that the constraint $\hat{C}_0^\dagger$ dictates.

The next term in the perturbation expansion gives

$$(\psi|^{(2)}\hat{C}_0^\dagger + (\psi|^{(0)}\Big(\sum_n \hat{C}_2^n\Big)^\dagger = 0. \tag{4.13}$$

This relation tells us that $\psi^{(2)}$ must satisfy a difference equation similar to that for $(\psi|^{(0)}$, but now with a source term which accounts for the interaction of the inhomogeneities with the "background" state $(\psi|^{(0)}$. Again, this can be interpreted as an evolution equation in the internal time v, in which any solution emerges out of the initial section without the need for any boundary condition around it. Consequently, if the initial data $\psi^{(2)}|_{v=\varepsilon}$ is provided, one can straightforwardly determine $\psi^{(2)}|_{v=\varepsilon+4}$ once $(\psi|^{(0)}$ is supplied: one only needs to solve a (well-posed) linear difference equation in v. By the same arguments, following an iterative process we can find the value of the solution on any other section $v = \varepsilon + 4n$, $\forall n \in \mathbb{N}$. In conclusion, any solution $(\psi|$ to the constraint can be determined if the initial data on the minimum volume section $(v = \varepsilon)$ are given. Although the construction of the solutions is formal, in general, we will see that this suffices to determine a physical Hilbert space which retains all the true degrees of freedom of the system.

To do that, we will proceed in a similar way as we did for the homogeneous part of the model in Sec. II B. Again, the important point is the fact that we can identify solutions with their initial data on the minimum volume section. Therefore, we just need to equip that space of initial data with a suitable inner product in order to construct the physical Hilbert space (see Ref. [13] for additional discussion). This inner product can be fixed, for instance, by demanding reality conditions on a complete set of observables [30]. Implementing this approach, the physical Hilbert space that we obtain is then

$$\mathcal{H}^{\text{phys}} = \mathcal{H}^{\text{kin}}_{\text{mat}} \otimes \mathcal{F}. \tag{4.14}$$

V. AN ALTERNATE GAUGE FIXING

In addition to the previous analysis, we will consider now an alternate gauge fixing in which the spatial metric looks homogeneous (and hence also the spatial curvature). We will carry out the reduction and quantization of the system in a similar way to what we did in the gauge discussed so far.

Let us start again with the constraint given in Eqs. (3.9), (3.10), and (3.11). We will impose the conditions $a_n = 0$ and $b_n = 0$, which are second class with the linear constraints. The stability of this gauge under the evolution can be ensured by fixing g_n and k_n as certain linear functions of the momenta π_{a_n} and π_{b_n}, whereas these momenta can be written as functions of the variables f_n and π_{f_n} –and the homogeneous variables– once the constraints $H^n_{|1} = 0$ and $H^n_{\_1} = 0$ are satisfied exactly.

Specifically, requiring that $\{b_n, \mathbb{H}\} = 0$, we arrive again at the very same condition given in Eq. (3.13), while (together with this last equation) the consistency demand $\{a_n, \mathbb{H}\} = 0$ leads to

$$g_n = \frac{1}{\pi_\alpha}\left(\frac{n^2-1}{n^2-4}\pi_{b_n} - \pi_{a_n}\right), \tag{5.1}$$

where we are using the following relations, obtained in the reduction process:

$$\begin{aligned} \pi_{a_n} &= \frac{\pi_\varphi}{\pi_\alpha}\pi_{f_n} + \frac{\tilde{m}^2 e^{6\alpha}\varphi}{\pi_\alpha} f_n, \\ \pi_{b_n} &= \frac{\pi_\varphi}{\pi_\alpha}\pi_{f_n} + \left(\frac{\tilde{m}^2 e^{6\alpha}\varphi}{\pi_\alpha} - 3\pi_\varphi\right) f_n. \end{aligned} \tag{5.2}$$

After introducing these last expressions in Eq. (3.9), we arrive at a Hamiltonian constraint of the same type as in Eq. (3.21), but with the new coefficients

$$\begin{aligned} E^n_{\pi\pi} &= 1 + \frac{3}{n^2-4}\frac{\pi_\varphi^2}{\pi_\alpha^2}, \\ E^n_{f\pi} &= -6\frac{\pi_\varphi^2}{\pi_\alpha} + \frac{3}{n^2-4}\left(\frac{2e^{6\alpha}\tilde{m}^2\varphi\pi_\varphi}{\pi_\alpha^2} - \frac{6\pi_\varphi^2}{\pi_\alpha}\right), \\ E^n_{ff} &= e^{4\alpha}(n^2-1) + e^{6\alpha}\tilde{m}^2 + 9\pi_\varphi^2 - \frac{6e^{6\alpha}\tilde{m}^2\varphi\pi_\varphi}{\pi_\alpha} \\ &\quad + \frac{3}{n^2-4}\left(3\pi_\varphi - \frac{e^{6\alpha}\tilde{m}^2\varphi}{\pi_\alpha}\right)^2. \end{aligned} \tag{5.3}$$

It is evident from all these equations that the introduced gauge fixing is always well posed except on the section of phase space corresponding to vanishing momentum π_α. We will see later that even the potential problems posed on that section are eluded in our quantization, owing to our regularization prescription and the fact that the kernel of the quantum counterpart of π_α belongs to the continuum spectrum, so that its corresponding operator can be inverted via the spectral theorem [34].

We will now introduce a scaling of the configuration variables f_n by the FRW scale factor, extended to a complete canonical transformation, so that the new canonical pair of fields that describe the matter perturbation admit a Fock quantization with the good properties explained in Sec. III C. To this end, in addition to the scaling of the f_n's, we perform the inverse scaling of the conjugate momenta, to which we also add a term linear in their corresponding configuration field variables in order to ensure that the cross-term coefficients $E^n_{f\pi}$ have a subdominant contribution to the matter field dynamics in the large n limit. Of course, we must transform the homogeneous variables as well, so that the entire transformation on phase space is canonical at the considered perturbative order. Explicitly, the canonical change is given by

$$
\begin{aligned}
\bar{\alpha} &= \alpha + \frac{1}{2}\left(1 - 3\frac{\pi_\varphi^2}{\pi_\alpha^2}\right)\epsilon^2 \sum_n f_n^2,\\
\bar{\pi}_\alpha &= \pi_\alpha + \epsilon^2 \sum_n \left[\left(3\frac{\pi_\varphi^2}{\pi_\alpha} + \pi_\alpha\right) f_n^2 - f_n \pi_{f_n}\right],\\
\bar{\varphi} &= \varphi + 3\frac{\pi_\varphi}{\pi_\alpha}\epsilon^2 \sum_n f_n^2, \qquad \bar{\pi}_\varphi = \pi_\varphi,\\
\bar{f}_n &= e^{\alpha} f_n, \quad \bar{\pi}_{f_n} = e^{-\alpha}\left[\pi_{f_n} - \left(3\frac{\pi_\varphi^2}{\pi_\alpha} + \pi_\alpha\right) f_n\right]. \quad (5.4)
\end{aligned}
$$

Under this transformation, the homogeneous part of the Hamiltonian constraint (3.8) is kept formally the same, though with the old homogeneous variables replaced with their new counterparts, whereas, in terms of the new inhomogeneous variables, the contributions quadratic in the perturbations have again the general form given by Eq. (3.24), but now with coefficients

$$
\begin{aligned}
\bar{E}^n_{\pi\pi} &= 1 + \frac{3}{n^2-4}\frac{\bar{\pi}_\varphi^2}{\bar{\pi}_\alpha^2},\\
\bar{E}^n_{f\pi} &= \frac{6}{e^{2\bar{\alpha}}(n^2-4)}\left(\frac{e^{6\bar{\alpha}}\tilde{m}^2\bar{\varphi}\bar{\pi}_\varphi}{\bar{\pi}_\alpha^2} - \frac{2\bar{\pi}_\varphi^2}{\bar{\pi}_\alpha} + \frac{3\bar{\pi}_\varphi^4}{\bar{\pi}_\alpha^3}\right),\\
\bar{E}^n_{ff} &= n^2 - 1 - \frac{1}{2e^{4\bar{\alpha}}}\left(\bar{\pi}_\alpha^2 - 30\bar{\pi}_\varphi^2 + \frac{27\bar{\pi}_\varphi^4}{\bar{\pi}_\alpha^2} - e^{4\bar{\alpha}}\right)\\
&\quad + e^{2\bar{\alpha}}\tilde{m}^2 - \frac{3e^{2\bar{\alpha}}}{2}\tilde{m}^2\bar{\varphi}\left[\frac{8\bar{\pi}_\varphi}{\bar{\pi}_\alpha} - \bar{\varphi}\left(\frac{3\bar{\pi}_\varphi^2}{\bar{\pi}_\alpha^2} - 1\right)\right] - \frac{3\bar{\pi}_\varphi^2}{2\bar{\pi}_\alpha^2}\\
&\quad + \frac{3}{e^{4\bar{\alpha}}(n^2-4)}\left(\frac{e^{6\bar{\alpha}}\tilde{m}^2\bar{\varphi}}{\bar{\pi}_\alpha} - 2\bar{\pi}_\varphi + \frac{3\bar{\pi}_\varphi^3}{\bar{\pi}_\alpha^2}\right)^2. \qquad (5.5)
\end{aligned}
$$

Finally, let us consider the variables c, p, ϕ, and p_ϕ applied in the quantization of the homogeneous system, already described in Sec. II. Again, they are given by Eqs. (3.5) and (3.6), replacing the old variables with their barred counterparts. Once more, we can combine a polymeric quantization of this homogeneous sector together with a standard Fock quantization of the inhomogeneities, providing a kinematical arena for the quantum treatment of the system. Following the quantization prescription of Sec. IV B, the reduced Hamiltonian constraint, with coefficients given by Eq. (5.5), can be promoted to an adequate operator, like the one introduced in Eq. (4.6) and with a similar contribution (4.7) of the inhomogeneities, but now with the operators

$$
\begin{aligned}
\hat{F}^n_\pm &= -\frac{3\sigma^2 l_0}{2}\left[m^2|\hat{p}|^{1/2}\left(-4\gamma(\hat{\phi}\hat{p}_\phi + \hat{p}_\phi\hat{\phi})\widehat{\Theta}^o_{(-1)} - \frac{3}{4}\gamma^2\sigma^2 l_0^3(\hat{\phi}\hat{p}_\phi + \hat{p}_\phi\hat{\phi})^2\widehat{\Theta}^e_{(-1)} + \hat{\phi}^2\right)|\hat{p}|^{1/2} + \gamma^2 l_0^2\hat{p}_\phi^2\widehat{\Theta}^e_{(-1)}\right]\\
&\quad + \frac{\sigma^2 l_0}{2}\widehat{\left[\frac{1}{V}\right]}^{2/3}\left(30\hat{p}_\phi^2 - 27\gamma^2\sigma^2 l_0^3\hat{p}_\phi^4\widehat{\Theta}^e_{(-1)} - \frac{\widehat{\Theta}^e_{(1)}}{\gamma^2 l_0^3\sigma^2}\right)\widehat{\left[\frac{1}{V}\right]}^{2/3} + \frac{3\sigma^2 l_0}{n^2-4}\widehat{\left[\frac{1}{V}\right]}^{2/3}\left(2\hat{p}_\phi + \gamma m^2|\hat{p}|^{3/2}\widehat{\Theta}^o_{(-1)}|\hat{p}|^{3/2}\hat{\phi}\right.\\
&\quad \left. - 3\gamma^2\sigma^2 l_0^3\hat{p}_\phi^3\widehat{\Theta}^e_{(-1)}\right)^2\widehat{\left[\frac{1}{V}\right]}^{2/3} + \frac{1}{2} + \frac{m^2}{l_0^2}\hat{p} \mp 3\sigma^2 l_0^3\gamma^2\frac{n^2-1}{n^2-4}\hat{p}_\phi^2\widehat{\Theta}^e_{(-1)}, \qquad (5.6)\\
\hat{G} &= 2\gamma l_0^2\widehat{\left[\frac{1}{V}\right]}^{1/3}\left[\frac{\gamma m^2}{2}(\hat{\phi}\hat{p}_\phi + \hat{p}_\phi\hat{\phi})|\hat{p}|^{3/2}\widehat{\Theta}^e_{(-1)}|\hat{p}|^{3/2} + 2\hat{p}_\phi^2\widehat{\Theta}^o_{(-1)} - 3\gamma^2\sigma^2 l_0^3\hat{p}_\phi^4|\hat{p}|^{1/2}\widehat{\Theta}^o_{(-2)}|\hat{p}|^{1/2}\right]\widehat{\left[\frac{1}{V}\right]}^{1/3}.
\end{aligned}
$$

This Hamiltonian constraint also decouples the zero volume state (tensor product any state on the matter field, both for its homogeneous part and its inhomogeneities), and is a combination of operators that preserve the superselection sectors of the homogeneous sector: semilattices of step 4 in the label v. On the other hand, notice the appearance of negative powers of $\hat{\Omega}^2$ through the terms $\widehat{\Theta}^o_{(-1)}$, $\widehat{\Theta}^o_{(-2)}$, and $\widehat{\Theta}^e_{(-1)}$. This inverse powers are well defined via the spectral decomposition of $\hat{\Omega}^2$, since the kernel of this operator is in its continuum spectrum [35].

Physical states are annihilated by the operator $\hat{C}$. We will assume the same perturbative form for them as in Eq. (4.11) (at the order studied in our approximation). The part $(\psi|^{(0)}$ of the solutions represents again a background-like state. Following the analysis carried out in Sec. II, any such solution (at zeroth perturbative order) is characterized by its initial data on the minimum volume section. Once that background solution is determined, one can evaluate $(\psi|^{(2)}$, which takes into account the interplay between the inhomogeneities and the homogeneous background. In Sec. IV C we saw that this part of the solution can be completely determined from its initial data at $v = \varepsilon$ once $(\psi|^{(0)}$ is known, at least formally. In total, we conclude that the space of solutions to the constraint $\hat{C}$ can be identified with the space of data on the minimum volume section. Finally, we can select a convenient inner product on this space, e.g., by choosing a complete set of observables and demanding that the complex conjugation relations between their elements become adjointness relations between their corresponding operators. In this way, we reach the same conclusion as in Sec. IV C: the physical Hilbert space can be taken unitarily equivalent to the Hilbert space (4.14).

VI. GAUGE-INVARIANT FORMULATION: A UNITARY MAP

Gauge-invariant quantities provide a physically meaningful description of cosmological perturbations [21]. Such quantities are usually employed to describe the physics in a consistent manner, independent of the identification of the spacetime and its matter content when transformations under diffeomorphisms are allowed, and insensitive to the specification of a particular gauge. In order to consolidate our proposal and show the robustness in this respect, in this section we will establish the correspondence between our fundamental variables $\bar{f}_n$ and $\bar{\pi}_{f_n}$ and gauge-invariant quantities, thus reformulating our quantum description in terms of the latter. Furthermore, we will see that both formulations (namely, the original one in terms of the matter field perturbations and the new one in terms of gauge invariants) are related by a canonical transformation which can be implemented quantum mechanically as a unitary transformation, at least, after deparametrization of the theory (e.g., in the regime of quantum field theory in a curved background spacetime).

Let us consider a transformation of the general type $x'^{\mu} = x^{\mu} + \epsilon\xi^{\mu}$, where x^{μ} is a spacetime point, ξ^{μ} is an arbitrary vector, and x'^{μ} is the transformed point (again, ϵ is the perturbative parameter introduced in Sec. III A). We express the covariant counterpart of ξ^{μ} using (hyper-)spherical harmonics, obtaining the mode expansion

$$\xi_0 = \sigma^2 N_0 \sqrt{2}\pi \sum_n \xi_0^n Q^n, \tag{6.1}$$

$$\xi_a = \sigma^2 e^{\alpha} \sqrt{2}\pi \sum_n \xi^n P_a^n. \tag{6.2}$$

On the other hand, instead of following the procedure presented in Ref. [11] to obtain gauge-invariant canonical pairs, here we will rather start from the standard formalism of Ref. [21], where several gauge-invariant perturbations are defined. In particular, we will consider the gauge-invariant quantities Φ_n^A, Φ_n^B, $\mathcal{E}_n^m$, and v_n^s given by Eqs. (C3)-(C6) of Appendix C. The first couple of invariants is constructed purely out of geometrical quantities. The second one contains also matter perturbations, and we will refer to them as the energy density and the velocity gauge-invariant perturbations, respectively. Any other gauge-invariant variable can be expressed as a linear combination of these four ones. This is the case of the Mukhanov-Sasaki variable (see Appendix D), which is a gauge-invariant perturbation *well adapted to flat scenarios*, where it satisfies the equation of motion of a scalar field propagating in a static spacetime but with a time-dependent potential (see, e.g., Ref. [11] for a recent discussion). However, for the matter content considered in this article, the gauge-invariant energy $\mathcal{E}_n^m$ (up to a suitable scaling) is more convenient inasmuch as it satisfies the same type of equation but independently of the spatial topology, a fact that makes it privileged in comparison with other invariants.

In fact, one can check that the combination of Eqs. (C11) and (C12) with (C16) and (C17) yields a system of first order differential equations for the quantities $\mathcal{E}_n^m$ and v_n^s which resembles the first order equations of a canonical pair of variables describing an oscillator with time-dependent frequency. Taking these considerations as our starting point, we define the following variables

$$\Psi_n = \frac{e^{5\alpha}}{\pi_\varphi\sqrt{n^2-4}} E_0 \mathcal{E}_n^m,$$
$$\Pi_{\Psi_n} = -\frac{\sqrt{n^2-4}}{\sqrt{n^2-1}} \frac{\pi_\varphi}{e^{\alpha}} v_n^s + \left(\frac{e^{6\alpha}\tilde{m}^2\varphi}{\pi_\varphi} - 2\pi_\alpha\right) \times \frac{e^{3\alpha}}{\pi_\varphi\sqrt{n^2-4}} E_0 \mathcal{E}_n^m. \tag{6.3}$$

Using Hamilton's equations for π_φ and α, one can actually see that the two introduced variables are related dynamically by

$$\dot{\Psi}_n = \Pi_{\Psi_n}, \tag{6.4}$$

where the dot stands for the derivative with respect to the conformal time (corresponding to $N_0 = e^{\alpha}$). With the above equation of motion and the corresponding one for $\dot{\Pi}_{\Psi_n}$, one obtains a second order differential equation for Ψ_n that corresponds exactly to that of the modes of a scalar field propagating in a static spacetime with a time-dependent quadratic potential.

In the rest of this section, we will show that, for each of the two gauge fixations considered in our discussion, the pair of gauge invariants defined in Eq. (6.3) are related with the fundamental fields $\bar{f}_n$ and $\bar{\pi}_{f_n}$ by means of a canonical transformation. Moreover, we will also prove that such a canonical transformation is implementable as a unitary transformation in the corresponding (deparametrized) quantum theory.

A. Longitudinal gauge $b_n = \Pi_n = 0$

In Sec. III we analyzed this gauge and introduced a canonical pair of variables $\bar{f}_n$ and $\bar{\pi}_{f_n}$, given in Eq. (3.23), to describe the inhomogeneities after the corresponding reduction of the system. If we now substitute these variables in expressions (C8) and (C10), and then in Eq. (6.3), we arrive at the following relations:

$$\Psi_n = \frac{1}{\sqrt{n^2-4}}(\bar{\pi}_{f_n} + \chi_A \bar{f}_n), \tag{6.5}$$
$$\Pi_{\Psi_n} = \frac{\chi_A}{\sqrt{n^2-4}}(\bar{\pi}_{f_n} + \chi_A \bar{f}_n) - \sqrt{n^2-4}\bar{f}_n,$$

where

$$\chi_A = e^{4\alpha}\tilde{m}^2 \frac{\varphi}{\pi_\varphi} - 2\frac{\pi_\alpha}{e^{2\alpha}} \tag{6.6}$$

only depends on the homogeneous variables. Notice also that, at the perturbative order of our approximation, the substitution in the above relations of the homogeneous variables α, π_α, φ, and π_φ by their barred counterparts appearing in Eq. (3.23) is totally irrelevant.

The change (6.5) can be regarded as a Bogoliubov transformation once we consider the creation and annihilation-like variables associated with each pair of variables, given by Eq. (4.1) and

$$b_n^\Psi = \frac{1}{\sqrt{2\omega_n}}(\omega_n \Psi_n + i\Pi_{\Psi_n}), \tag{6.7}$$

together with the complex conjugate. A simple calculation allows us to compute the coefficients associated with the antilinear part of this Bogoliubov transformation:

$$\beta_n = \frac{i}{2}\frac{\chi_A^2 + 3}{\sqrt{n^2-1}\sqrt{n^2-4}}. \tag{6.8}$$

In order to determine whether the transformation admits or not a unitary implementation, the necessary and sufficient condition is just that

$$\sum_{nlm} |\beta_n|^2 = \sum_n d_n |\beta_n|^2 < \infty, \tag{6.9}$$

where d_n is a degeneracy factor accounting for the dimension of each eigenspace of the Laplace-Beltrami operator. Explicitly, we have on the three-sphere that $d_n = n^2$. As a result, the canonical transformation between our variables $\bar{f}_n$ and $\bar{\pi}_{f_n}$, and the gauge-invariant ones, Ψ_n and Π_{Ψ_n}, turns out to be implementable as a unitary one at the quantum level, since the coefficients β_n are clearly square summable, including their degeneracy. Therefore, the two considered physical descriptions are completely equivalent.

B. Gauge $a_n = b_n = 0$

Let us now consider the gauge fixing carried out in Sec. V. Again, one can find the relation in the reduced system between the canonical pair $\bar{f}_n$ and $\bar{\pi}_{f_n}$ and the gauge invariants Ψ_n and Π_{Ψ_n}. For this, one can first obtain the expressions of $\mathcal{E}_n^m$ and v_n^s in terms of $\bar{f}_n$ and $\bar{\pi}_{f_n}$ (in the gauge under consideration) and then use Eq. (6.3). A simple calculation yields an expression similar to Eq. (6.5), but substituting χ_A by

$$\chi_B = e^{4\alpha}\tilde{m}^2 \frac{\varphi}{\pi_\varphi} - 2\frac{\pi_\alpha}{e^{2\alpha}} + 3\frac{\pi_\varphi^2}{e^{2\alpha}\pi_\alpha}. \tag{6.10}$$

We can then compute the corresponding β-coefficients of the Bogoliubov transformation relating the creation and annihilation-like variables associated with the variables $\bar{f}_n$ and $\bar{\pi}_{f_n}$, on the one hand, and the gauge-invariant variables, on the other hand. The result is the same as in Eq. (6.8), but now with χ_B replacing χ_A. Following the arguments of Sec. VI A, we can easily check the unitary implementability of this Bogoliubov transformation, since condition (6.9) holds.

VII. SUMMARY AND CONCLUSIONS

In this article, we have presented the quantization of an inflationary universe with small inhomogeneities. The matter content is described by a minimally coupled, massive scalar field. First, we have studied the corresponding symmetry-reduced homogeneous and isotropic system in Sec. II. In order to employ a polymeric quantization [4] for the geometry degrees of freedom, its classical phase space has been parametrized by a densitized triad and an Ashtekar-Barbero connection. As for the (homogeneous) matter content, we have applied a standard Schrödinger quantization. In this kinematical arena, we have introduced an operator representation for the Hamiltonian constraint. The geometric part of this quantum constraint is a difference operator that only relates states with support in semilattices with points separated by constant steps of four units. Additionally, these semilattices can be characterized by a continuous, non-vanishing parameter $\varepsilon \in (0, 4]$, which is proportional to the minimum physical volume allowed in the quantum theory on that semilattice. Moreover, we have argued that every sector of the kinematical Hilbert space with support on any of those semilattices is superselected. As any physical state belongs to the kernel of the constraint, one can see that the restriction to a particular superselection sector allows us to entirely determine any solution if its initial data on the minimum volume section are provided. The final step to quantize the system to completion, i.e., to construct the physical Hilbert space, is to equip the space of solutions with an adequate inner product. Based on the identification of the space of solutions with the space of initial data for minimum volume, we have picked up this inner product by selecting a complete set of observables and imposing reality conditions on them [30], namely, by requiring that the complex conjugation relations in this set become adjointness relations between the operators which represent the observables. Our proposal allows us not only to formalize the quantization of the system, but also to proceed in the analysis of its quantum dynamics. The extension of the systematic procedures commonly used in LQC to systems without an explicit separation of the matter content from the geometry is not obvious, yet our proposal sheds new insights to confront also those more general situations. Our preliminary numerical analysis shows that, with an appropriate choice of initial data, it is possible to recover physical states that represent an expanding universe preceded by a contracting one with a well-defined quantum bounce connecting both of them, even for a massive scalar field. Those results are very promising and a more careful study will be the subject of future research.

On the other hand, to progress in the applicability of LQC to the analysis of the Early Universe and construct a quantum framework to study the development of small inhomogeneities in inflationary scenarios, we have introduced local degrees of freedom in our model by means of perturbation theory around the homogeneous and isotropic solutions. We have concentrated our efforts in the understanding of scalar perturbations, because of the fundamental role that they play in present observational cosmology. Additionally, from the technical point of view, scalar modes are more involved than vector or tensor ones, since they incorporate both physical and gauge degrees of freedom and their discrimination is not trivial. In order to distinguish the true physical degrees of freedom, we have carried out two different partial gauge fixings. The first one is the so-called longitudinal gauge, commonly used in standard cosmology, and the second one is the natural gauge fixing in which the spatial metric is purely homogeneous (i.e., all the inhomogeneities of the metric are encoded in the perturbations of the lapse and shift functions). In both cases, we reach a description of the inhomogeneities of the corresponding reduced system in terms of the matter perturbations. We have introduced a canonical transformation in each case, with an eye on the standard Fock quantization of the inhomogeneities, quantization that we have carried out later on. Such a new choice of canonical fields is motivated by the recent uniqueness results regarding the quantization of linear fields (generically) in non-stationary spacetimes [25], where the choice of a Fock quantum theory with a vacuum state invariant under the spatial isometries and unitary dynamics selects privileged canonical field variables for the description of the system, together with a specific quantum representation for such field variables. We have then adopted this Fock representation for the inhomogeneities and combined it with the polymeric description initially introduced in Sec. II B.

Furthermore, we have presented a quantization prescription for the Hamiltonian constraint in Sec. IV B. The corresponding quantum operator respects the superselection sectors of the homogeneous setting. Therefore, any state which is a solution to the constraint has support in semilattices of constant step in the physical volume, starting from a non-vanishing minimum value of it. We have been able to prove that, assuming that the solutions to the constraint admit an expansion in terms of the perturbative parameter ϵ, the lowest order contribution in the perturbative expansion of a solution can be regarded as a background state, in which the inhomogeneities play no dynamical role, and which can be totally determined by its initial data on the volume section $v=\varepsilon$. On the other hand, it can be seen that the next contribution in the expansion of the solution satisfies the FRW constraint equation but with a source term coming from the interaction of the inhomogeneities and the background state. Again, we have proven that this contribution to the solution can be determined once its initial data on the minimum volume section are provided. Therefore, in order to construct the physical Hilbert space, we just have to endow the space of initial data for the solutions with a Hilbert space structure, supplying it with an inner product which, for instance, can be selected by requiring reality conditions on a complete set of observables defined on the section $v=\varepsilon$. The very same procedure has been carried out in Sec. V for the alternate gauge fixing considered in this article.

In addition, to avoid any gauge-fixing dependence of the possible physical outcomes of our proposals, we have introduced a family of gauge-invariant variables. We have constructed a canonical pair of conjugate variables out of the gauge-invariant energy and velocity perturbations (see Ref. [21] and Appendix C). Adopting a standard Fock description for them (namely, the so-called massless representation), we have been able to prove that the fundamental matter perturbations in each (gauge-fixed) reduced system and the new gauge-invariant variables are related by means of a canonical transformation that can be implemented unitarily quantum mechanically. Moreover, the uniqueness results of Ref. [25] can be immediately applied to the gauge-invariant variables proposed in this article. Therefore, the physics predicted by the different descriptions proposed in this work (either based on gauge invariants or not) is equivalent, at least as far as standard quantum field theory in curved spacetimes is concerned.

In conclusion, we have been able to provide a full quantum description of an inflationary universe with small inhomogeneities propagating on it, in the context of LQC. The model is now ready to produce physical predictions, which will be the aim of future work.

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Appendix A: Unitary transformation

In this Appendix, we will provide a unitary transformation that cancels the complex phases in the definition of the operator $\widehat{\Omega}^2$ constructed from Eq. (2.4). This operator is given by

$$\widehat{\Omega}^2 = -\hat{N}_{2\bar{\mu}}\hat{R}_{+}(v)\hat{R}_{-}^{\dagger}(v)\hat{N}_{2\bar{\mu}} - \hat{N}_{-2\bar{\mu}}\hat{R}_{-}(v)\hat{R}_{+}^{\dagger}(v)\hat{N}_{-2\bar{\mu}} + (|\hat{R}_{+}(v)|^2 + |\hat{R}_{-}(v)|^2), \tag{A1}$$

where

$$R_{\pm}(v) = \frac{\pi\gamma G\hbar}{2}|v|^{1/2}|v\pm 2|^{1/2}\left[\mathrm{sgn}(v)+\mathrm{sgn}(v\pm 2)\right] \times e^{\mp i l_0\left(\frac{\bar{\mu}(v)}{2}+\frac{\bar{\mu}(v\pm 2)}{2}\right)}, \tag{A2}$$

and $\bar{\mu}(v) = [\Delta/(2\pi\gamma G\hbar v)]^{1/3}$.

Given a generic function $h(v)$, we define its complex exponentiation

$$\hat{U} = e^{i l_0 \hat{h}(v)}. \tag{A3}$$

We consider now the operator $\hat{U}\widehat{\Omega}^2\hat{U}^{-1}$ and, in particular, the $\hat{N}_{4\bar{\mu}}$ term (the contribution of $\hat{N}_{-4\bar{\mu}}$ is given by the adjoint, and the remaining part of $\widehat{\Omega}^2$ is a multiplicative operator in the v-representation). We can see that the complex phases cancel if, $\forall v$,

$$h(v+2) - h(v-2) = \frac{\bar{\mu}(v+2)}{2} + \frac{\bar{\mu}(v-2)}{2} + \bar{\mu}(v). \tag{A4}$$

Let us change the label $v \to v+2$ and restrict the transformation to a superselection sector with, e.g., positive orientation of the triad, i.e., $v = \varepsilon + 4n$ ($n \in \mathbb{N}$), without loss of generality. Then, we are able to determine the explicit form of the function $h(v)$ by a recursive process:

$$\begin{aligned}
h(\varepsilon) &= \frac{\bar{\mu}(\varepsilon)}{2}, \\
h(\varepsilon+4) &= \frac{\bar{\mu}(\varepsilon+4)}{2} + \bar{\mu}(\varepsilon+2) + \frac{\bar{\mu}(\varepsilon)}{2} + h(\varepsilon) \\
&= \frac{\bar{\mu}(\varepsilon+4)}{2} + \bar{\mu}(\varepsilon+2) + \bar{\mu}(\varepsilon), \\
h(\varepsilon+8) &= \frac{\bar{\mu}(\varepsilon+8)}{2} + \bar{\mu}(\varepsilon+6) + \frac{\bar{\mu}(\varepsilon+4)}{2} + h(\varepsilon+4) \\
&= \frac{\bar{\mu}(\varepsilon+8)}{2} + \bar{\mu}(\varepsilon+6) + \bar{\mu}(\varepsilon+4) + \bar{\mu}(\varepsilon+2) + \bar{\mu}(\varepsilon), \\
h(\varepsilon+4n) &= \frac{\bar{\mu}(\varepsilon+4n)}{2} + \sum_{j=0}^{2n-1}\bar{\mu}(\varepsilon+2j), \ n\in\mathbb{N}^{+}.
\end{aligned} \tag{A5}$$

The constraint $\hat{C}$, involving the operator $\widehat{\Omega}^2$, superselects sectors. Once the analysis is restricted to a specific sector, it is natural to introduce in it a unitary transformation of the above form. In this sector, the operator $\widehat{\Omega}^2$ is then mapped into $\widehat{\Omega}_0^2$ [see Eq. (2.6)]. It is worth commenting that, for large n, the function $h(v)$ converges to the function $v^{2/3}$ (up to a factor), essentially because the sum in (A5) converges to the integral $\int dv\, v^{-1/3} \sim v^{2/3}$ and the first term in that expression is $\bar{\mu}(v) \sim o(v^{-1/3})$. Therefore, we recover the function of the corresponding unitary map introduced in Ref. [4].

Appendix B: (Hyper-)Spherical harmonics

We now briefly summarize the main properties of the (hyper-)spherical harmonics Q^n_{lm} on S^3 [31, 36]. They form a basis (of square integrable functions with respect to the volume element defined by the standard metric on the three-sphere) in which the Laplace-Beltrami operator is diagonal, with a discrete and unbounded negative spectrum. They are labeled with three integers: n, l, and m. The last two account for the degeneracy of each eigenvalue of the Laplace-Beltrami operator. Their ranges are $0 \le l \le n-1$ and $-l \le m \le l$. We will display these labels explicitly only in those steps of our analysis in which they play a relevant role.

Thus, the scalar harmonics Q^n are eigenfunctions of the Laplace-Beltrami operator on S^3, and specifically they satisfy

$$Q^n{}_{|a}{}^{|a} = -(n^2-1)Q^n, \quad n = 1,2,3... \tag{B1}$$

Here, the symbol $|$ denotes the covariant derivative with respect to the round metric Ω_{ab} on the three-sphere of unit radius. Since we deal with real scalar fields in our discussion, we choose the harmonics Q^n to be *real*.

Starting from these scalar harmonics, it is straightforward to construct a family of vector harmonics P^n_a by applying covariant derivatives:

$$P^n_a = \frac{1}{n^2-1}Q^n{}_{|a}, \quad n = 2,3,4.... \tag{B2}$$

These vector harmonics satisfy

$$P^n_a{}_{|b}{}^{|b} = -(n^2-3)P^n_a, \quad P^{n|a}_a = -Q^n. \tag{B3}$$

In addition, we can also construct a family of tensor harmonics, namely, the scalar tensors

$$Q^n_{ab} = \frac{1}{3}\Omega_{ab}Q^n, \quad n = 1,2,3..., \tag{B4}$$

and the traceless tensors

$$P^n_{ab} = \frac{1}{n^2-1}Q^n{}_{|ab} + \frac{1}{3}\Omega_{ab}Q^n, \quad n = 2,3,4... \tag{B5}$$

These traceless tensors have the following properties

$$P^{n}_{ab|c}{}^{|c} = -(n^2-7)P^n_{ab},$$
$$P^{n}_{ab}{}^{|b} = -\frac{2}{3}(n^2-4)P^n_a,$$
$$P^{n}_{ab}{}^{|ab} = \frac{2}{3}(n^2-4)Q^n. \tag{B6}$$

Finally, if we call dv the integration measure on S^3 corresponding to the volume element determined by the metric Ω_{ab}, and we normalize the scalar harmonics so that

$$\int dv\, Q^n_{lm}Q^{n'}_{l'm'} = \delta_{nn'}\delta_{ll'}\delta_{mm'}, \tag{B7}$$

it is straightforward to check that

$$\int dv (P_a)^n_{lm}(P^a)^{n'}_{l'm'} = \frac{1}{n^2-1}\delta_{nn'}\delta_{ll'}\delta_{mm'},$$
$$\int dv (Q_{ab})^n_{lm}(Q^{ab})^{n'}_{l'm'} = \frac{1}{3}\delta_{nn'}\delta_{ll'}\delta_{mm'},$$
$$\int dv (P_{ab})^n_{lm}(P^{ab})^{n'}_{l'm'} = \frac{2}{3}\frac{n^2-4}{n^2-1}\delta_{nn'}\delta_{ll'}\delta_{mm'}. \tag{B8}$$

Appendix C: Bardeen potentials

In this appendix, we provide the definitions of some relevant gauge-invariant quantities [21] and discuss the dynamical relations between them. In doing this, we use the expansion of the metric components and the matter field given in Eqs. (3.1)-(3.4). We consider gauge transformations of the form $x'^{\mu} = x^{\mu} + \epsilon\xi^{\mu}$, introduced in Sec. VI, with the parametrization (6.1) and (6.2).

After a transformation of this kind, the modes of the metric can be written in terms of the original ones and the modes of ξ_μ:

$$g_n \mapsto g_n + \frac{1}{e^\alpha}\dot{\xi}^n_0, \tag{C1}$$
$$k_n \mapsto k_n - \frac{N_0}{e^\alpha}\left(\omega_n^2\xi^n_0 + \dot{\xi}^n - \dot{\alpha}\xi^n\right),$$
$$a_n \mapsto a_n + \frac{1}{e^\alpha}\left(\frac{1}{3}\xi^n + \dot{\alpha}\xi^n_0\right),$$
$$b_n \mapsto b_n - \frac{1}{3e^\alpha}\xi^n,$$
$$f_n \mapsto f_n + \frac{\dot{\varphi}}{e^\alpha}\xi^n_0. \tag{C2}$$

Recall that the overdot stands for the derivative with respect to the conformal time η, and $\omega_n^2 = n^2-1$. With these transformation rules, the following scalar modes define gauge-invariant quantities:

$$\Phi^A_n = g_n + \frac{1}{e^\alpha\omega_n^2}\frac{d}{d\eta}\left(\frac{e^\alpha}{N_0}k_n - 3e^\alpha\dot{b}_n\right), \tag{C3}$$
$$\Phi^B_n = a_n + b_n + \frac{\dot{\alpha}}{\omega_n^2}\left(\frac{k_n}{N_0} - 3\dot{b}_n\right), \tag{C4}$$
$$\mathcal{E}^m_n = \frac{1}{E_0 e^{2\alpha}}\left[\dot{\varphi}\dot{f}_n - \dot{\varphi}^2 g_n + (3\dot{\alpha}\dot{\varphi} + e^{2\alpha}\tilde{m}^2\varphi)f_n\right] \tag{C5}$$
$$v^s_n = \frac{1}{\omega_n}\left(\frac{\omega_n^2}{\dot{\varphi}}f_n + \frac{k_n}{N_0} - 3\dot{b}_n\right), \tag{C6}$$

where $E_0 = (e^{-2\alpha}\dot{\varphi}^2 + \tilde{m}^2\varphi^2)/2$ is proportional to the energy density of the background scalar field. If we compare these quantities with the gauge-invariant variables originally defined in Ref. [21], we see that the gauge-invariant Φ^A can be identified with the potential defined in Eq. (3.9) of that reference. On the other hand, the Bardeen potential defined in Eq. (3.10) of that work corresponds to the quantity Φ^B. Our invariant energy density perturbation, $\mathcal{E}^m$, is the gauge invariant of Bardeen's Eq. (3.13). Finally, the gauge-invariant matter velocity of Eq. (3.11) in Ref. [21] corresponds to v^s.

Let us derive now the expressions of $\mathcal{E}^m_n$ and v^s_n as functions of the canonical variables introduced in Sec. III. For the gauge-invariant energy density and velocity perturbations, we need to employ the dynamical equations in order to rewrite the momenta π_{f_n} and π_{b_n} in terms of the time derivative of the corresponding conjugate variables, i.e., $\dot{f}_n$ and $\dot{b}_n$, respectively. For the matter perturbation we obtain

$$\pi_{f_n} = e^{2\alpha}\dot{f}_n + \pi_\varphi(3a_n - g_n). \tag{C7}$$

Taking this into account, a simple computation yields

$$\mathcal{E}^m_n = \frac{1}{E_0 e^{6\alpha}}\left[\pi_\varphi\left(\pi_{f_n} - 3\pi_\varphi a_n\right) + \left(e^{6\alpha}\tilde{m}^2\varphi - 3\pi_\varphi\pi_\alpha\right)f_n\right]. \tag{C8}$$

On the other hand, for the momentum conjugate to b_n we have

$$\pi_{b_n} = \frac{n^2-4}{n^2-1}\left(e^{2\alpha}\dot{b}_n - 4\pi_\alpha b_n - \frac{1}{3}e^{2\alpha}\frac{k_n}{N_0}\right). \tag{C9}$$

Therefore, the velocity gauge-invariant perturbation can be written as

$$v^s_n = \frac{1}{\omega_n}\left[\frac{e^{2\alpha}}{\pi_\varphi}\omega_n^2 f_n - \frac{3}{e^{2\alpha}}\left(\frac{n^2-1}{n^2-4}\pi_{b_n} + 4\pi_\alpha b_n\right)\right]. \tag{C10}$$

We now turn to the relations existing between these gauge-invariant quantities. On the one hand, one can check that the equation of motion for the perturbation b_n (see Eq. (B11) of Ref. [31]) is equivalent to

$$\Phi^A_n + \Phi^B_n = 0, \quad n = 3, 4\ldots \tag{C11}$$

This equation corresponds to Eq. (4.4) in Ref. [21], valid for any fluid whose stress-energy tensor has a vanishing traceless part. Another interesting relation arises from a linear combination of the constraints $H^n_{|1}$ and $H^n_{\_1}$, given in Eqs. (3.10) and (3.11), respectively. One can see that

$$H^n_{|1} - 3\dot{\alpha}H^n_{\_1} - 3H_{|0}a_n = e^{3\alpha}E_0\mathcal{E}^m_n - \frac{1}{3}e^{\alpha}(n^2-4)\Phi^B_n.$$

If the conditions $H^n_{|1} = 0$ and $H^n_{\_1} = 0$ are satisfied, the last equation reduces to Eq. (4.3) of Ref. [21], or, equivalently,

$$\Phi^B_n = \frac{3e^{2\alpha}}{n^2-4}E_0\mathcal{E}^m_n. \tag{C12}$$

Let us now define

$$P_0 = \frac{1}{2}\Big(\frac{\dot{\varphi}^2}{e^{2\alpha}} - \tilde{m}^2\varphi^2\Big), \quad w = \frac{P_0}{E_0}, \tag{C13}$$

$$c_s^2 = \frac{dP_0}{dE_0} = 1 + \frac{2e^{2\alpha}\tilde{m}^2\varphi}{3\dot{\alpha}\dot{\varphi}}, \tag{C14}$$

$$\eta_n = \frac{\delta P_n}{P_0} - \frac{dP_0}{dE_0}\frac{\delta E_n}{P_0} = \frac{1-c_s^2}{w}\mathcal{E}^m_n. \tag{C15}$$

Here, P_0 is proportional to the pressure of the homogeneous matter field, while δE_n and δP_n are the modes of the energy-density and pressure perturbations. Using these formulas, one straightforwardly proves that Eq. (4.5) of Ref. [21] can be written as

$$E_0\mathcal{E}^m_n = \frac{\dot{\varphi}^2}{e^{3\alpha}}\left[\frac{1}{\omega_n}\frac{d}{d\eta}(e^{\alpha}v^s_n) - e^{\alpha}\Phi^A_n\right]. \tag{C16}$$

Finally, we can obtain an energy equation like Eq. (4.8) of Ref. [21]. We start from the equation of motion of f_n, which is a second-order differential equation that can be found in Eq. (B14) of Ref. [31]. If we combine it with Eqs. (C11) and (C12), and with the equation of motion of α, we arrive at the expression

$$\frac{d}{d\eta}\left(e^{3\alpha}E_0\mathcal{E}^m_n\right) = -\frac{n^2-4}{n^2-1}e^{\alpha}\dot{\varphi}^2\omega_n v^s_n. \tag{C17}$$

Appendix D: Gauge-invariant curvature perturbation

Another interesting gauge-invariant quantity is the curvature perturbation, which is defined as

$$\mathcal{R}_n = \Phi^B_n - \frac{\dot{\alpha}}{\omega_n}v^s_n, \tag{D1}$$

and was originally studied by Bardeen (see the corresponding definition in Eq. (5.19) of Ref. [21]). In the case of *spatially flat cosmologies*, it is common to work with a closely related quantity, the so-called Mukhanov-Sasaki variable $v_n = z\mathcal{R}_n$, with $z = e^{\alpha}\dot{\varphi}/\dot{\alpha}$. In such situations, the power spectrum of primordial perturbations can be easily derived using the Mukhanov-Sasaki variable.

In our case, this gauge invariant has different expressions in terms of the canonical variables employed in the two distinct gauge fixings considered here.

a. Longitudinal gauge

In order to compute $\mathcal{R}_n$ in terms of our fundamental fields $\bar{f}_n$ and $\bar{\pi}_{f_n}$, we recall first that the potential Φ^B_n is related with $\mathcal{E}^m_n$ by means of Eq. (C12). Applying the results of Sec. VI, it is then easy to obtain that

$$\mathcal{R}_n = \frac{3\pi_\varphi}{e^{3\alpha}(n^2-4)}(\bar{\pi}_{f_n} + \chi_A\bar{f}_n) + \frac{\pi_\alpha}{e^{\alpha}\pi_\varphi}\bar{f}_n. \tag{D2}$$

The variable χ_A was defined in Eq. (6.6). Clearly, in the large n limit, the main contribution to the previous expression comes from the last factor, proportional to $\bar{f}_n$.

b. Gauge fixing $a_n = b_n = 0$

This gauge provides a simple relation between the curvature perturbation and the modes $\bar{f}_n$. Actually, using the definitions (D1), (C4), and (C6), a straightforward computation yields

$$\mathcal{R}_n = \frac{\pi_\alpha}{e^{\alpha}\pi_\varphi}\bar{f}_n. \tag{D3}$$

Therefore, in this gauge, where the spatial geometry is homogeneous, the unique contribution to the curvature perturbation comes essentially from the perturbation of the scalar field.

Moreover, in the ultraviolet limit, the form of the curvature perturbation coincides formally with that of the longitudinal gauge, given by Eq. (D2). As a consequence, for the two studied gauges, the Mukhanov-Sasaki variable v_n either coincides with $\bar{f}_n$ (gauge $a_n = b_n = 0$) or converges to it (longitudinal gauge).

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[33] As we will discuss in Sec. VI, even when the results of Ref. [25] pick up a particular pair of canonical fields among those related by the considered class of time-dependent canonical transformations, more general canonical transformations can in principle be implemented unitarily as well, e.g., in cases in which we may allow them to have a suitable mode dependence.

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