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Combining loop and Fock quantizations for cosmological universes with perturbations

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A complete quantization of an approximately homogeneous and isotropic universe with small scalar perturbations and compact flat spatial topology is carried out by means of a hybrid approach in Loop Quantum Cosmology. The matter content is provided by a minimally coupled massive scalar field. The homogenous sector of the geometry degrees of freedom is polymerically quantized, while the inhomogeneities are quantized employing Fock techniques. The Fock quantization adopted is a privileged one, picked out in a unique way by criteria of dynamical unitarity and symmetry invariance in the context of quantum field theory in curved space-times. We characterize the physical states of this quantum theory and investigate some aspects of the resulting physics, including the connection with standard cosmological perturbation theory.

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1. Introduction and outline

It is generally accepted that the universe that we observe is approximately homogeneous in an appropriate range of large scales, and isotropic in the sense that no direction is preferential, as confirmed by the temperature distribution of the cosmic microwave background (CMB) (and theoretically supported by the EGS theorem for certain matter contents [1]). This homogeneous and isotropic universe on average can be described by a Friedmann-Robertson-Walker (FRW) cosmology, totally characterized by the type of curvature of the spatial sections seen by comoving observers (namely, a positive, zero, or negative curvature, corresponding to elliptic, Euclidean, or hyperbolic geometry, respectively) and by a scale factor that changes in the comoving time and dictates the modification experienced in distances. The large scale structures seen in our universe, as well as the anisotropies detected in the CMB, are thought to have originated in inhomogeneities of the primordial universe generated by quantum fluctuations of the geometry and matter fields. These inhomogeneities are usually considered sufficiently small as to allow their treatment as perturbations, superposed to the FRW background [2]. The standard explanation to the generation of these inhomogeneities in a way consistent with observations is based on a mechanism of inflation, which drove the evolution of the universe to a fast and large expansion in a very short period of the early cosmological history [3].

Probably, the simplest model that can generate a satisfactory inflation is a universe with a matter content consisting of a massive scalar field, at least for a certain range of values of the mass (which do not include the massless case). In this model, the field is just a scalar, with no internal structure, and its potential is just the mass term, therefore quadratic in the field, simplifying the study enormously while retaining sufficient complexity to make the model interesting. We will consider a minimal coupling for the field, ignoring other possible but more complicated couplings. In addition, we will discuss the case in which the spatial topology of the FRW background is flat. This topology is the simplest to deal with from the operational viewpoint, since the field equations do not include then contributions of the spatial curvature. But, more importantly, flat topology is picked out as the preferred case by cosmological observations [4]. The effects of spatial curvature can be studied, e.g., by considering spherical topology [5], case from which the flat one can be recovered essentially by disregarding the corresponding curvature terms in the gravitational action. On the other hand, we do not only assume flat spatial sections, but also compact ones. The compactness does not affect the cosmological observations if the size of the compact universe is, let's say, much larger than the Hubble horizon, since physics beyond that scale should not be relevant for cosmological phenomena. From the viewpoint of quantum field theory in a cosmological background, compactness allows us to avoid infrared problems, related to the existence of an infinite number of perturbative modes infinitesimally close to the global, zero modes of the system.

Given its physical interest and simplicity, this model has been repeatedly studied in the literature of quantum cosmology (usually with non-flat topology [6, 7]) to discuss the kind of quantum processes that might leave an imprint in the primordial perturbations. Nonetheless, up to recent years the system had not been studied in the framework of Loop Quantum Cosmology (LQC) [8]. The revisited analysis is particularly important both because of the rigorous control gained with the probabilistic interpretation of the quantum theory in LQC, which provides solid fundamentals to the predictions, and because of the good properties exhibited by the quantum evolution of

FRW models in the application of Loop Quantum Gravity (LQG) [9] to cosmology [10, 11, 12]. In particular, the Big Bang singularity is resolved quantum mechanically and replaced with a Big Bounce, a process in which the contraction/expansion of the universe bounces owing to repulsive effects of the quantum geometry. Through this bouncing mechanism, our branch of the universe connects with another previous branch that was in contraction. Both branches keep their semiclassical behavior for sufficiently well peaked quantum states of the geometry, but nonetheless depart from the dynamics of general relativity in the regions of large matter density, close to the bounce [12, 13].

In fact, this system and other models related to cosmological perturbations have been studied in the context of LQC following an approach that does not face its direct quantization. Instead, most of those analyses were based on the modified algebra of constraints obtained by assuming certain types of loop corrections and demanding the absence of anomalies for consistency. From this modified algebra, new field equations for the perturbations were derived and the corresponding consequences for the CMB discussed [14]. On the other hand, other studies have started from an extrapolation of the effective dynamics associated with LQC, extending conclusions about this effective description in homogeneous cosmologies to systems with inhomogeneities [15]. In contrast, in order to deal with the cosmological perturbations, we will carry out a complete quantization of the system. This is especially interesting, since it provides a way to reach predictions from basic principles and obtain results from which one may, in particular, try and check the validity of the assumptions employed in other kinds of approaches. For this aim, it is important that we perform as few approximations as possible in our treatment, and that we keep those approximations under control. Besides, those approximations ought to be deduced from general considerations, or at least be checked eventually to confirm their self consistency in our formalism. In this sense, we note that it is not always possible to prove the validity of some approximations, because one would need a fully general and well posed theory from which one could derive the demonstration. Since this is not the case, not only in LQC, but also in LQG, the best that one can frequently do is to check the self consistency in the proposed formulation, within the introduced approximation.

With this motivation in mind, we will discuss the quantization of scalar perturbations around an FRW cosmology with a minimally coupled massive scalar field and a three-torus spatial topology [16]. The first approximation that we will use is to truncate the gravitational action (in Hamiltonian form) at quadratic order in the inhomogeneous perturbations. This truncation is similar to that performed in the canonical formulation of quantum cosmology by Halliwell and Hawking [6]. The truncation scheme allows us to maintain backreaction effects on the background, exactly up to the perturbative order in the action here considered. Keeping this quadratic order in the action is essential for self consistency, as we will see. Moreover, the fact that all quadratic perturbative terms are maintained leads to a description that is more general than other less refined truncations discussed very recently in the literature [17, 18]. Hence, our approach would allow us to analyze regimes in which those other truncations can be reached, and investigate their range of applicability.

The other approximation that we will employ in our quantization is the so-called hybrid approach within LQC. The hybrid approach is a hierarchy to the quantization of the geometry, in which one assumes that the most relevant quantum effects are those affecting the background. In this way, one adopts a polymeric quantization of the degrees of freedom of the background geometry, using loop techniques, and combines this quantum treatment with a more standard, Fock quantization of the perturbations. The fact that one can combine these two types of quantization techniques is not trivial, because the different degrees of freedom are coupled (at least) by the Hamiltonian constraint. Nevertheless, the hybrid program has been applied successfully [19] in the study of Gowdy cosmologies (cosmologies with inhomogeneities that depend only on one spatial direction) [20], and its use for cosmological perturbations has been developed in Refs. [5, 16, 21, 22]. It is worth remarking that the hybrid quantization of Gowdy models does not require any perturbative truncation of the gravitational action: in that case, the treatment is exact, and no truncation is needed, since the action is already quadratic in the field variables adopted for the system. This provides even more robustness to the results obtained for Gowdy universes. In our case, both the hybrid approach and the quadratic truncation of the action are necessary to handle with the problem.

In carrying out this hybrid quantization, an important issue is the choice of a specific field description for the inhomogeneous perturbations as well as a concrete Fock representation for the corresponding canonical commutation relations (CCR's). This is of the most relevance, because in cosmological scenarios a part of the time dependence of the inhomogeneous fields can be attributed to the background, therefore affecting the selection of field description and changing the corresponding field dynamics. Furthermore, even assuming that a specific canonical pair has been picked out for each field, one has in principle infinitely many possible Fock representations of the corresponding CCR's. The physical ambiguity in this choice can be viewed as the freedom in the selection of a specific vacuum (which involves a particular concept of particle, associated with it) [23]. There exists an infinite number of inequivalent choices, each of them leading to different physical predictions. This would ruin the robustness of the quantum description, since one would have infinitely many physical outcomes at hand, while only one universe is available to compare the predictions with observations. This ambiguity, typical of quantum field theory in curved space-times, is removed in simple cases by appealing to background symmetries. For instance, in Minkowski space-time, one demands the vacuum to be invariant under the Poincaré symmetries of the background. In stationary space-times, where a well-defined notion of energy is available, one can remove the infinite ambiguity in the choice of Fock representation with requirements about the energy of the quantum field [24]. Nevertheless, generally these kinds of symmetry conditions are not sufficient in non-stationary scenarios. In such situations, where there is still spatial symmetry remaining in the background, but time symmetries are absent, it seems natural to keep the demands of invariance under the persisting symmetries, as well as to replace the lost time invariance with the requirement of a unitary implementation of the evolution in the Fock quantization. Notice that this unitarity permits a standard probabilistic interpretation of the quantum theory. Recent results [25, 26] prove that, indeed, the combined criteria of (i) invariance under the spatial symmetries of the field equations, and (ii) implementability of the quantum dynamics as a unitary transformation, select a unique class of equivalent Fock representations, and thus remove the physical ambiguity in the quantization. Moreover, the above requirements suffice in fact to choose only one canonical pair among all those that are related by time-dependent canonical transformations that involve a scaling of the field configuration (absorbed by assigning that part of the time dependence to the background) [26, 27]. In this way, one arrives at a well justified separation between the degrees of freedom of the inhomogeneous fields and those of the background. Let us comment that other recent works on cosmological perturbations in LQC do not include this specific scaling that makes the dynamics unitarily implementable [17, 18]. Obviously, this affects the quantum description, and in particular the effective approaches therein derived.

Moreover, one can even consider non-local canonical transformations, respecting the decoupling of the field modes of the inhomogeneous perturbations [28]. This kind of non-local transformations relate, for instance, the perturbative degrees of freedom in gauge-fixed formulations with the gauge invariants that describe those degrees [21]. Again, the uniqueness of the Fock quantization, up to unitary equivalence, is guaranteed by our criteria of imposing spatial symmetry invariance and unitary dynamics.

The rest of this work is organized as follows. We first present the classical description of the model, using Ashtekar-Barbero variables for the FRW geometry [8] and annihilation and creation-like variables for the perturbations. We then fix gauge in the system, eliminating all but one of the non-physical (canonical pairs of) degrees of freedom. The reduced model has only one global, Hamiltonian constraint. We also comment on the robustness of our study under changes of gauge, and on the use of gauge invariants for the perturbations. Next, we proceed to quantize the reduced model employing a hybrid approach. Our final step consists in obtaining solutions to the constraint, showing that one regains a standard quantum field theory for the perturbations under certain approximations. Finally, we summarize our results and conclude.

2. The classical model

For the classical description of our system, we choose variables that are especially suitable to pass to the hybrid quantization of the model in a quite straightforward way. Thus, we use Ashtekar-Barbero variables to describe the geometry of the FRW background. The matter content of this background is given by the zero mode, in a Fourier expansion, of the massive scalar field. Finally, for the inhomogeneities, we employ also a decomposition in Fourier modes on the spatial sections. These modes are eigenfunctions of the corresponding Laplace-Beltrami (LB) operator of the flat metric on the three-torus.

The Ashtekar-Barbero variables are a su(2) connection A_a^i and a densitized triad E_i^a [9]. Latin letters from the beginning and the middle of the alphabet denote, respectively, SU(2) and spatial indices, taking values from 1 to 3. We choose angular spatial coordinates $\vec{\theta}$ on the three-torus, each of them with period equal to 2π. The densitized triad contains the information about the spatial metric, whereas the connection is classically equivalent to the sum of the spin connection compatible with the triad plus the extrinsic curvature expressed in triadic form. In this sum, actually, the extrinsic curvature can be multiplied by any positive constant γ. This constant is usually called the Immirzi parameter [29]. Taking into account the homogeneity and isotropy of the model, it is not difficult to realize that, with an appropriate choice of SU(2) gauge, the Ashtekar-Barbero variables can be written in the form

$$A_a^i = c\,\frac{{}^0e_a^i}{2\pi}, \qquad E_i^a = p\left|{}^0e\right|\frac{{}^0e_i^a}{(2\pi)^2}, \tag{2.1}$$

where ${}^0e_a^i$ is a fiducial triad of reference, e.g. the standard diagonal flat triad ${}^0e_a^i = \delta_a^i$, $\left|{}^0e\right|$ is its determinant, c and p are two geometry variables (evolving in time) with canonical Poisson brackets, $\{c,p\} = 8\pi G\gamma/3$, and G is Newton constant. We notice that, as a consequence, the degrees of freedom contained in the Ashtekar-Barbero variables reduce just to the canonical pair

c and p. The relation of this pair with the scale factor a of the FRW model (or rather with its logarithm α) and with the corresponding momentum is

$$a^2 = e^{2\alpha} = \frac{|p|}{(2\pi\sigma)^2}, \qquad \pi_\alpha = -\frac{pc}{\gamma 8\pi^3\sigma^2}. \tag{2.2}$$

Here, we have introduced the constant $\sigma^2 = G/(6\pi^2)$. On the other hand, to describe the homogeneous part of the massive scalar field, we will use a canonical pair, ϕ and π_ϕ, which denote its configuration and conjugate momentum. Their Poisson bracket is equal to 1. To simplify our formulas, it will also prove convenient to introduce a scaled canonical pair, differing from the former by a constant factor:

$$\varphi = (2\pi)^{3/2}\sigma\phi, \qquad \pi_\varphi = \frac{\pi_\phi}{(2\pi)^{3/2}\sigma}. \tag{2.3}$$

If we now define the volume variable $V = |p|^{3/2}$, proportional to the volume of the spatial sections of the FRW model with three-torus topology, a straightforward calculation shows that the only constraint on the system in the completely homogeneous situation (without any inhomogeneous perturbation), namely the homogeneous Hamiltonian constraint, would be

$$C_0 = -\frac{6}{\gamma^2}\sqrt{|p|}c^2 + \frac{8\pi G}{V}(\pi_\phi^2 + m^2V^2\phi^2). \tag{2.4}$$

The constant m is the mass of the scalar field.

Let us now consider the inhomogeneities. Since the massive scalar field Φ (which includes perturbations, in contrast to the homogenous part ϕ) satisfies a Klein-Gordon equation, where all the spatial dependence appears via the action of the LB differential operator, it is natural to use a basis of eigenfunctions of this operator to expand the inhomogeneities. These eigenfunctions form just a basis of Fourier modes. We choose them real, in order to incorporate the reality of the scalar field in a simple way in the corresponding Fourier expansion. Since we are only interested in describing the inhomogeneous contributions, we exclude the zero mode from this expansion, which is already taken into account in the canonical pair ϕ and π_ϕ. The orthonormalized Fourier basis is composed of the cosine and sine functions (denoted with a subindex $+$ and $-$, respectively):

$$Q_{\vec{n},+} = \frac{1}{2\pi^{3/2}}\cos\vec{n}\cdot\vec{\theta}, \qquad Q_{\vec{n},-} = \frac{1}{2\pi^{3/2}}\sin\vec{n}\cdot\vec{\theta}. \tag{2.5}$$

The notation $\vec{n}$ stands for any non-vanishing tuple of integers in which the first non-zero component is positive. This positivity restriction is introduced in order not to consider twice the same mode, since the sines and cosines change at most in a sign under a flip of sign in the tuple. The above functions are eigenmodes of the LB operator of the standard flat metric on the three-torus, with eigenvalue $-\omega_n^2 = -\vec{n}\cdot\vec{n}$. Note that there exists degeneracy in each eigenspace, not only owing to flips of signs and permutations in the components of the tuples, but also accidental degeneracy in some cases.

In our discussion, we will only consider scalar perturbations in the space-time metric. This is totally consistent inasmuch as scalar perturbations are decoupled from vector and tensor perturbations of the metric at the adopted quadratic order of truncation in the action [6]. We describe the metric in a 3+1 decomposition [30] in terms of the spatial metric h_{ij}, induced on the sections of constant time with three-torus topology (with fiducial flat metric given by ${}^0h_{ij}$), the lapse function, and the shift vector. Then, the combined form of the homogenous contributions and the inhomogeneous scalar perturbations to the metric and the scalar field can be expressed as

$$
\begin{aligned}
h_{ij} &= (\sigma e^{\alpha(t)})^2 \left[{}^0h_{ij} + 2\varepsilon(2\pi)^{3/2} \sum \left\{ a_{\vec{n},\pm}(t) Q_{\vec{n},\pm} {}^0h_{ij} + b_{\vec{n},\pm}(t) \left(\frac{3}{\omega_n^2} (Q_{\vec{n};\pm})_{;ij} + Q_{\vec{n},\pm} {}^0h_{ij} \right) \right\} \right], \\
N &= \sigma N_0(t) \left[1 + \varepsilon(2\pi)^{3/2} \sum g_{\vec{n},\pm}(t) Q_{\vec{n},\pm} \right], \\
N_i &= \varepsilon(2\pi)^{3/2} \sigma^2 e^{\alpha(t)} \sum \frac{k_{\vec{n},\pm}(t)}{\omega_n^2} (Q_{\vec{n},\pm})_{;i}, \\
\Phi &= \frac{1}{\sigma} \left[\frac{\varphi(t)}{(2\pi)^{3/2}} + \varepsilon \sum f_{\vec{n},\pm}(t) Q_{\vec{n},\pm} \right].
\end{aligned}
\tag{2.6}
$$

The covariant derivative with respect to ${}^0h_{ij}$ is here denoted with a semicolon. The homogeneous part of the lapse function is $\sigma N_0(t)$. The parameter ε is a perturbative parameter, introduced for convenience in order to track the perturbative order of the expressions more easily. The time dependent coefficients $a_{\vec{n},\pm}$, $b_{\vec{n},\pm}$, $g_{\vec{n},\pm}$, $k_{\vec{n},\pm}$, and $f_{\vec{n},\pm}$ characterize the perturbations. The variables $a_{\vec{n},\pm}$ and $b_{\vec{n},\pm}$ describe, respectively, the trace and traceless contributions of the perturbations to the spatial metric. The coefficients $g_{\vec{n},\pm}$ and $k_{\vec{n},\pm}$ provide the perturbations of the lapse and the shift, and therefore are expected not to correspond to physical degrees of freedom. Finally, the inhomogeneities of the scalar field are given by the variables $f_{\vec{n},\pm}$.

If one substitutes these expressions in the gravitational action and truncates it at quadratic order in perturbations, after a lengthy but trivial calculation one arrives at the following total Hamiltonian for the perturbed system, formed by a linear combination of constraints:

$$
H = \frac{N_0\sigma}{16\pi G} C_0 + \varepsilon^2 \sum \left(N_0 H_2^{\vec{n},\pm} + N_0 g_{\vec{n},\pm} H_1^{\vec{n},\pm} + k_{\vec{n},\pm} \widetilde{H}_1^{\vec{n},\pm} \right). \tag{2.7}
$$

We thus confirm that $g_{\vec{n},\pm}$ and $k_{\vec{n},\pm}$ appear as Lagrange multipliers, accompanying the linear perturbative (scalar and diffeomorphisms) constraints $H_1^{\vec{n},\pm}$ and $\widetilde{H}_1^{\vec{n},\pm}$, respectively. Besides, we see that the zero mode of the scalar constraint, for which N_0 is the Lagrange multiplier, acquires now a quadratic contribution in the perturbations, provided by $\sum H_2^{\vec{n},\pm}$. The exact form of the perturbative constraints can be found in Ref. [16].

3. Gauge fixing

We can now proceed to eliminate non-physical degrees of freedom by fixing the gauge corresponding to the linear perturbative constraints. We will adopt the longitudinal gauge, in which the three-metric is conformally flat and the shift vector vanishes. This gauge fixing is employed frequently in the literature. Since $k_{\vec{n},\pm}$ are just Lagrange multipliers, we cannot use the requirement that they vanish directly as gauge-fixing conditions. To make the shift equal to zero we must impose a suitably chosen restriction on the dynamical variables of the system. As in Refs. [5, 16], the appropriate conditions for the longitudinal gauge are

$$
\pi_{a_{\vec{n},\pm}} - \pi_\alpha a_{\vec{n},\pm} - 3\pi_\varphi f_{\vec{n},\pm} = 0, \qquad b_{\vec{n},\pm} = 0. \tag{3.1}
$$

When these equations are imposed, the constraint $\widetilde{H}_1^{\vec{n},\pm}=0$ implies that $\pi_{b_{\vec{n},\pm}}=0$, while $H_1^{\vec{n},\pm}=0$ leads to

$$a_{\vec{n},\pm}=3\frac{\pi_\varphi\pi_{f_{\vec{n},\pm}}+\left(e^{6\alpha}m^2\sigma^2\varphi-3\pi_\alpha\pi_\varphi\right)f_{\vec{n},\pm}}{9\pi_\varphi^2+\omega_n^2e^{4\alpha}}. \tag{3.2}$$

To arrive at this relation, third-order terms in the perturbations have been neglected. On the other hand, the dynamical consistency of the conditions (3.1) requires in fact that the shift vector vanish, as we wanted.

In the reduction of the system, after imposing the gauge-fixing conditions, the non-zero value of the terms of the form $\dot{a}_{\vec{n},\pm}\pi_{a_{\vec{n},\pm}}$ in the Lagrangian (where the dot denotes the time derivative) leads to a contribution to the action when one removes the canonical pairs $(a_{\vec{n},\pm},\pi_{a_{\vec{n},\pm}})$ as physical degrees of freedom. One can see that, as a consequence, the Poisson brackets of the remaining variables change [16]. A new set of canonical coordinates after reduction, at the perturbative order of truncation in the action, is

$$\begin{aligned}
&\bar{\varphi}=\varphi+3\varepsilon^2\sum a_{\vec{n},\pm}f_{\vec{n},\pm}, && \pi_{\bar{\varphi}}=\pi_\varphi,\\
&\bar{\alpha}=\alpha+\tfrac{\varepsilon^2}{2}\sum\left(a_{\vec{n},\pm}^2+f_{\vec{n},\pm}^2\right), && \pi_{\bar{\alpha}}=\pi_\alpha-\varepsilon^2\sum f_{\vec{n},\pm}\left(\pi_{f_{\vec{n},\pm}}-3\pi_\varphi a_{\vec{n},\pm}-\pi_\alpha f_{\vec{n},\pm}\right),\\
&\bar{f}_{\vec{n},\pm}=e^\alpha f_{\vec{n},\pm}, && \pi_{\bar{f}_{\vec{n},\pm}}=e^{-\alpha}(\pi_{f_{\vec{n},\pm}}-3\pi_\varphi a_{\vec{n},\pm}-\pi_\alpha f_{\vec{n},\pm}).
\end{aligned} \tag{3.3}$$

In particular, we see that the genuine background variables get corrections that are quadratic in the perturbations. Notice also that we have already scaled the matter field variables $f_{\vec{n},\pm}$ by the FRW scale factor, to adopt the field description that is selected by the requirement that, in the context of quantum field theory in a curved space-time, the dynamics of the reduced system can admit a unitary implementation under a Fock quantization (invariant under the spatial isometries).

The dynamics of the reduced system is such that the modes of the scaled matter field satisfy an equation of Klein-Gordon type with time-dependent mass:

$$\ddot{\bar{f}}_{\vec{n},\pm}+r_n\dot{\bar{f}}_{\vec{n},\pm}+(\omega_n^2+s+s_n)\bar{f}_{\vec{n},\pm}=0, \tag{3.4}$$

with a canonical momentum of the form

$$\pi_{\bar{f}_{\vec{n},\pm}}=(1+p_n)\dot{\bar{f}}_{\vec{n},\pm}+q_n\bar{f}_{\vec{n},\pm}, \tag{3.5}$$

where we have used the notation

$$s=m^2\sigma^2e^{2\bar{\alpha}}-\frac{e^{-4\bar{\alpha}}}{2}\left(\pi_{\bar{\alpha}}^2+21\pi_{\bar{\varphi}}^2+3e^{6\bar{\alpha}}m^2\sigma^2\bar{\varphi}^2\right), \tag{3.6}$$

and r_n, s_n, p_n, and q_n denote functions (of the corrected background variables) which are of order ω_n^{-2} in the LB eigenvalue [16]. This asymptotic order is sufficiently subdominant as to allow that the results of uniqueness about the Fock representation of our (scaled) matter field and its momentum continue to apply. Recall that this uniqueness (modulo unitary transformations) is guaranteed by the criteria of invariance under the isometries of the three-torus and the unitary implementability of the evolution [21].

Actually, the dynamical equation of the matter perturbations can be put in the exact form of a Klein-Gordon field equation with time-dependent mass, without mode-dependent modifications,

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by means of a canonical transformation that varies in time but which, nonetheless, is mode dependent. Hence this transformation is non-local from the viewpoint of the original scalar field. Even so, remarkably, it is possible to see that this canonical transformation turns out to be unitarily implementable in the Fock quantization selected by our criteria [28].

Only one constraint remains in the reduced model obtained after gauge fixing, which is the zero mode of the Hamiltonian constraint, again given by the Hamiltonian constraint of the background part of the system together with contributions of the perturbations:

$$H = \frac{N_0\sigma}{16\pi G}C_0 + \varepsilon^2 N_0 \sum H_2^{\vec{n},\pm}, \tag{3.7}$$

where the perturbative terms are quadratic in the inhomogeneous modes,

$$H_2^{\vec{n},\pm} 2e^{\bar{\alpha}} = \bar{E}_{\bar{f}\bar{f}} \bar{f}^2_{\vec{n},\pm} + \bar{E}_{\bar{f}\pi} \bar{f}_{\vec{n},\pm} \pi_{\bar{f}_{\vec{n},\pm}} + \bar{E}_{\pi\pi} \pi^2_{\bar{f}_{\vec{n},\pm}}. \tag{3.8}$$

The explicit form of the coefficients in this quadratic expression is

$$\begin{aligned} \bar{E}^n_{\bar{f}\bar{f}} &= \omega_n^2 + e^{2\bar{\alpha}} m^2 \sigma^2 - \frac{e^{-4\bar{\alpha}}}{2}\left(\pi^2_{\bar{\alpha}} + 15\pi^2_{\bar{\varphi}} + 3e^{6\bar{\alpha}} m^2\sigma^2\bar{\varphi}^2\right) - \frac{3e^{-8\bar{\alpha}}}{\omega_n^2}\left(e^{6\bar{\alpha}} m^2\sigma^2\bar{\varphi} - 2\pi_{\bar{\alpha}}\pi_{\bar{\varphi}}\right)^2, \\ \bar{E}^n_{\bar{f}\pi} &= -\frac{3e^{-6\bar{\alpha}}}{\omega_n^2}\pi_{\bar{\varphi}}\left(e^{6\bar{\alpha}} m^2\sigma^2\bar{\varphi} - 2\pi_{\bar{\alpha}}\pi_{\bar{\varphi}}\right), \\ \bar{E}^n_{\pi\pi} &= 1 - \frac{3e^{-4\bar{\alpha}}}{\omega_n^2}\pi^2_{\bar{\varphi}}. \end{aligned} \tag{3.9}$$

Finally, we have checked that the results obtained with other possible gauge choices are similar, a fact that shows the robustness of our conclusions beyond the selection of a specific gauge. For instance, we have repeated the reduction of the system in a gauge with flat spatial sections at all times. We have proven that the Fock quantization selected in that case by our criteria of spatial symmetry invariance and unitary evolution of the matter inhomogeneities is unitarily equivalent to the quantization constructed above in the longitudinal gauge. Moreover, we have related our mode variables for the matter inhomogeneities in our reduced model with the modes of the Mukhanov-Sasaki variable [31] and its momentum, which are gauge invariant quantities [32]. We have demonstrated that the canonical transformation that relates these two sets of variables is in fact unitarily implementable in our Fock quantization, therefore providing further support to our description.

4. Hybrid quantization

We can now carry out the hybrid quantization of our reduced system, using the so-called polymeric quantization of LQC [8] for the homogeneous sector of the model, and a Fock quantization for the infinite number of degrees of freedom corresponding to the Fourier modes of the inhomogeneities of the scalar field.

For our homogeneous sector, we will employ a specific prescription for the loop quantization which is known as the MMO proposal [33]. This particular prescription for the quantization has certain advantages while keeping essentially the same physics that appears in other prescriptions and which is behind the quantum resolution of cosmological singularities [10, 11, 12]. For

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instance, in the MMO proposal, the quantum evolution can be defined straightforwardly without the need to recur to ideal clocks (e.g., given by the homogenous component of a massless field). Besides, the Wheeler-DeWitt limit of the polymeric quantization of the FRW space-times is unambiguous with this prescription (in each superselection sector) [33]. Perhaps more importantly for practical purposes is the fact that the MMO proposal is optimal for numerical simulations, reducing considerably the computation time and the complexity of the codes [33].

Our homogeneous variables are defined in the first two lines of Eq. (3.3). In the following, we remove the over-bars in those variables in order to simplify our notation. We start by adopting a basis of volume eigenstates $\{|v\rangle; v \in \mathbb{R}\}$ of the operator $\hat{V} = |\hat{p}|^{3/2}$ [the relation of p with the variables used for the homogeneous FRW geometry is that given in Eq. (2.2)]. The polymeric quantization is characterized by a discrete inner product in this volume basis [8]:

$$\forall\, v_1, v_2 \in \mathbb{R}, \qquad \langle v_1 | v_2 \rangle = \delta^{v_1}_{v_2}. \tag{4.1}$$

In this representation, clearly, the volume acts by multiplication, and hence the triad as well, since it is just a function of the former. As for the connection, one considers the holonomies obtained by integrating it along edges. This line integrals characterize the connection faithfully, and are independent of SU(2) gauge transformations when the edges are made to close. In fact, in the homogenous situation that we are considering, it suffices to consider holonomies along (fiducial) straight edges: these holonomies contain all the relevant information. They take the expression

$$h_{^0 e_i}(\bar{\mu}) = \cos\left(\frac{\bar{\mu}c}{2}\right)\mathbf{1} + 2\sin\left(\frac{\bar{\mu}c}{2}\right)\tau_i, \tag{4.2}$$

where τ_i form a set of SU(2) generators and, apart from a factor of $-i/2$, can be identified with the Pauli matrices. The quantity $\bar{\mu}$ determines the fiducial length of the edge on which the holonomy has been calculated, and can take any real value. Therefore, we see that the elements of the relevant holonomies are linear combinations of the functions $N_{\bar{\mu}} = e^{i\bar{\mu}c/2}$.

The value of $\bar{\mu}$ is frequently chosen in LQC by demanding that the physical area enclosed by a square of edge with that fiducial length be equal to the area gap Δ, i.e., the minimum non-zero eigenvalue of the quantum area in LQG [34]. With this choice, usually called the improved dynamics prescription [12], the actions of the above holonomy elements and of the triad variable in the volume basis (with Planck constant denoted by $\hbar$) are given explicitly by [8]

$$\hat{N}_{\bar{\mu}}|v\rangle = |v+1\rangle, \qquad \hat{p}|v\rangle = \mathrm{sign}(v)\left(2\pi\gamma G\hbar\sqrt{\Delta}|v|\right)^{2/3}|v\rangle. \tag{4.3}$$

The kinematic Hilbert space of the polymeric representation for the homogeneous sector of the model, once we take into account not only the geometry, but also the zero mode of the massive scalar field, is the product $H^{FRW-LQC}_{kin} \otimes H^{matt}_{kin}$, where the first factor is the Hilbert space obtained for the FRW model in LQC by completing the span of our volume basis with the product (4.1), and the second factor is the Hilbert space, standard in quantum mechanics, of integrable square functions in the configuration variable of the homogeneous scalar field. In this representation space, the inverse volume is regularized as usual in LQC [8]:

$$\widehat{\left[\frac{1}{V}\right]} = \widehat{\left[\frac{1}{\sqrt{|p|}}\right]}^3, \qquad \widehat{\left[\frac{1}{\sqrt{|p|}}\right]} = \frac{3}{4\pi\gamma G\hbar\sqrt{\Delta}}\widehat{\mathrm{sign}(p)}\sqrt{|\hat{p}|}\left(\hat{N}_{-\bar{\mu}}\sqrt{|\hat{p}|}\hat{N}_{\bar{\mu}} - \hat{N}_{\bar{\mu}}\sqrt{|\hat{p}|}\hat{N}_{-\bar{\mu}}\right). \tag{4.4}$$

This operator has not only a well-defined action on the state of zero volume, a property behind the resolution of singularity problems in the loop quantum formulation, but, moreover, it turns out to annihilate that state. As a result, one can prove that the zero-volume state completely decouples from the rest of volume eigenstates after the imposition of the homogenous Hamiltonian constraint in the quantum theory [33]. This allows one to change the densitization of that constraint, simplifying the analysis. For the homogeneous sector, this change is provided by the correspondence

$$\hat{C}_0 = \widehat{\left[\frac{1}{V}\right]}^{1/2} \hat{\mathbf{C}}_0 \widehat{\left[\frac{1}{V}\right]}^{1/2}, \tag{4.5}$$

where

$$\hat{\mathbf{C}}_0 = -\frac{6}{\gamma^2}\hat{\Omega}_0^2 + 8\pi G\left(\hat{\pi}_\phi^2 + m^2\hat{\phi}^2\hat{V}^2\right) \tag{4.6}$$

and we have represented the gravitational part, according to the MMO proposal, by the operator

$$\hat{\Omega}_0 = \frac{1}{4i\sqrt{\Delta}}\hat{V}^{1/2}\left[\widehat{\text{sign}(p)}\left(\hat{N}_{2\bar{\mu}} - \hat{N}_{-2\bar{\mu}}\right) + \left(\hat{N}_{2\bar{\mu}} - \hat{N}_{-2\bar{\mu}}\right)\widehat{\text{sign}(p)}\right]\hat{V}^{1/2}. \tag{4.7}$$

Notice that we have used a symmetric factor ordering, algebraic in powers of V, and taken especial care of the sign of p, which determines the orientation of the triad in the Ashtekar-Barbero formalism.

The action of this geometry operator has the generic form

$$\widehat{\Omega}_0^2|v\rangle = f_+(v)|v+4\rangle + f_0(v)|v\rangle + f_-(v)|v-4\rangle. \tag{4.8}$$

In particular, this action superselects the Hilbert space $H_{kin}^{FRW-LQC}$, which is non-separable, into sectors that are separable independently. Each of these sectors contains volume states with eigenvalues that differ by a multiple of 4 units. Moreover, owing to the symmetrization in the sign of p made in Eq. (4.7), the real functions $f_+(v)$ and $f_-(v)$ vanish, respectively, in the whole interval [-4,0] and [0,4]. A a result, the action of the considered operator does not connect positive and negative eigenvalues of the volume. In total, the operator preserves the superselection sectors $\mathfrak{L}_{\pm\rho}^{(4)} := \{\pm(\rho+4n),\ n\in\mathbb{N}\}$, which are semilattices of points spaced by four units. Each of them is totally characterized by the point which is closer to the origin, which can be described by its sign and its absolute value ρ (which may run in (0,4]).

The geometry operator $\widehat{\Omega}_0^2$ that appears in the homogeneous constraint can be shown to be self-adjoint in each of these superselection sectors. Its eigenfunctions can be chosen to be real (since the functions f_0, f_+, and f_- turn out to be real) and are completely determined by their value at the minimum volume $\pm\rho$, which can be used as initial condition to integrate the eigenvalue difference equation associated with Eq. (4.8). Similarly, the quantum solutions to the complete homogeneous constraint can be constructed starting from their initial values on the section of minimum volume in the analyzed superselection sector. Consequently, one can identify the space of physical states with the space of those initial conditions endowed with a suitable Hilbert structure, so that the important observables of the homogenous sector become self-adjoint operators; for instance, one can choose the Hilbert space $L^2(\mathbb{R},d\phi)$. Alternatively, if one identifies the zero mode of the scalar field as an internal clock, one can integrate the quantum constraint in ϕ providing initial conditions for fixed value of this field configuration.

Let us discuss now the Fock quantization of the inhomogeneities of our system. We quantize the scaled inhomogeneous modes using annihilation and creation-like variables defined in terms of our canonical variables just as it would be natural to do in the case of zero mass. Namely, the chosen annihilation and creation-like variables are those whose frequency coincides with the eigenvalue of the LB operator [16]. In this way, it is straightforward to construct a Fock space $\mathfrak{F}$ with associated basis of n-particle states of the form

$$\left\{|N\rangle = |N_{(1,0,0),+}, N_{(1,0,0),-}, \ldots\rangle; \quad N_{\vec{n},\pm} \in \mathbb{N}, \; \sum N_{\vec{n},\pm} < \infty\right\}. \tag{4.9}$$

That is, for each element of this basis, the occupation number in each particle mode is a non-negative integer, and the sum of all those integers is finite.

The hybrid quantization is attained by adopting the product space $H_{kin}^{FRW-LQC} \otimes H_{kin}^{matt} \otimes \mathfrak{F}$ as representation space. The remaining, global Hamiltonian constraint has a non-trivial action on this space. To define it, we need to select a quantum representation of the term that contains quadratic contributions of the perturbations, namely $\sum H_2^{\vec{n},\pm}$. We do this by adopting the quantization proposals already explained for the homogeneous sector, using a symmetric factor ordering, and employing the Fock representation that has been selected, in the context of quantum field theory in curved space-times, by our criteria of spatial symmetry invariance and unitary dynamics [25]. In more detail: (1) we symmetrize products of the type $\hat{\phi}\hat{\pi}_\phi$; (2) we take a symmetric geometric factor ordering $V^k A \to \hat{V}^{k/2}\hat{A}\hat{V}^{k/2}$ for all products involving powers of V; (3) we adopt the LQC representation $(cp)^{2m} \to \left[\hat{\Omega}_0^2\right]^m$; and (4) in order to preserve the FRW superselection sectors, we adopt the prescription $(cp)^{2m+1} \to \left[\hat{\Omega}_0^2\right]^{m/2} \hat{\Lambda}_0 \left[\hat{\Omega}_0^2\right]^{m/2}$, where

$$\hat{\Lambda}_0 = -\frac{i}{8\sqrt{\Delta}}\hat{V}^{1/2}\left[\widehat{\mathrm{sign}(p)}\left(\hat{N}_{4\bar{\mu}} - \hat{N}_{-4\bar{\mu}}\right) + \left(\hat{N}_{4\bar{\mu}} - \hat{N}_{-4\bar{\mu}}\right)\widehat{\mathrm{sign}(p)}\right]\hat{V}^{1/2}. \tag{4.10}$$

This last prescription for the representation of cp, actually, is similar to that followed to represent the Hubble parameter in LQC, since otherwise its action would not leave invariant the superselection sectors of the FRW cosmology. The exact form of the constraint operator constructed in this manner can be consulted in Ref. [16].

5. Physical states

Once we have quantized our model of an FRW space-time with a massive scalar field and scalar perturbations, and after we have found a representation of the only constraint of the system in this quantum theory, we will investigate the solutions to that constraint, which provide the wave functions that describe the possible physical states.

First, let us accept that the matter field may serve as a clock. We can then consider positive (negative) frequency states with respect to that time, in particular in the restriction to the homogeneous sector of the model. For the complete system, we can concentrate our attention on states which satisfy an ansätz similar to the Born-Oppenheimer approximation of molecular physics [35]. This ansätz consists in a separation of the dependence of the wave function Ψ in homogeneous and inhomogeneous variables, using the homogeneous field configuration ϕ as an internal time:

$$\Psi = \chi_0(v,\phi)\,\psi(\phi, N[\bar{f}_{\vec{n},\pm}]). \tag{5.1}$$

We then assume that the variation of the inhomogeneous part in this internal time is negligible compared to that of the FRW part. Here, $N[\bar{f}_{\vec{n},\pm}]$ denotes the inhomogeneous variables of our Fock representation. Besides, $\chi_0(v,\phi)$ is taken as a (positive frequency) quantum solution to the homogeneous constraint, sufficiently peaked around a classical FRW solution for large values of the volume V as to guarantee the validity of the effective quantum dynamics of homogeneous LQC [15]. In other words, we can use effective LQC to describe the evolution of the peak. After a bit of calculus, one can show that the introduced ansätz and approximation lead to a sort of *effective* quantum field theory for the inhomogeneities [16]:

$$-i\hbar\partial_\phi\tilde{\psi} = \frac{\varepsilon^2}{2}\frac{\langle {}^{(0)}\hat{\Theta}_2 + {}^{(1)}\hat{\Theta}_2\hat{H}_0\rangle_{\chi_0}}{\langle\hat{H}_0\rangle_{\chi_0}}\tilde{\psi}, \tag{5.2}$$

where $\langle\,\rangle_{\chi_0}$ denotes the expectation value with respect to the FRW geometry [taking the inner product (4.1) of LQC], the operator $\hat{H}_0^2$ coincides with the square of the homogeneous field momentum modulo the homogeneous Hamiltonian constraint,

$$\hat{H}_0^2 = \hat{\pi}_\phi^2 - \frac{\hat{\mathbf{C}}_0}{8\pi G}, \tag{5.3}$$

we have scaled the wave function of the inhomogeneities:

$$\tilde{\psi} = \left[\langle\hat{H}_0\rangle_{\chi_0}\right]^{1/2}\psi, \tag{5.4}$$

and, finally, ${}^{(0)}\hat{\Theta}_2$ and ${}^{(1)}\hat{\Theta}_2$ are defined in terms of the quadratic contributions of the perturbations to the constraint, $\hat{H}_2^{\vec{n},\pm}$, as follows. First, we change the densitization of this term exactly as we did with the homogeneous term of the constraint:

$$\hat{H}_2^{\vec{n},\pm} = \frac{\sigma}{16\pi G}\left[\widehat{\frac{1}{V}}\right]^{1/2}\hat{\mathbf{C}}_2^{\vec{n},\pm}\left[\widehat{\frac{1}{V}}\right]^{1/2}. \tag{5.5}$$

Then, we split $\hat{\mathbf{C}}_2^{\vec{n},\pm}$ in contributions with odd and with even powers of $\hat{\pi}_\phi$. Using relation (5.3) to replace all integer powers of the square of the homogeneous field momentum by $\hat{H}_0^2$ at the studied perturbative level, and representing the remaining momentum $\hat{\pi}_\phi$ as $-i\hbar$ times the derivative with respect to ϕ, we define our operators $\hat{\Theta}_2$ by the equation

$$\sum\hat{\mathbf{C}}_2^{\vec{n},\pm} = -8\pi G\left({}^{(0)}\hat{\Theta}_2 - i\hbar\,{}^{(1)}\hat{\Theta}_2\partial_\phi\right). \tag{5.6}$$

Our formula (5.2) can be understood as a Schrödinger equation with physical Hamiltonian given on the right hand side. This Hamiltonian can be interpreted as the Mukhanov-Sasaki Hamiltonian for the inhomogeneities, expressed in terms of our variables, and evaluated at the homogeneous background determined by the peak of the FRW quantum state χ_0, whose evolution is ruled by effective LQC. Therefore, the corresponding background can be regarded as an FRW space-time dressed with (polymeric) quantum modifications.

If one does not want that the analysis of the physical states rests on the choice of any specific internal time, one can always adopt an alternate scheme, based on a perturbative expansion of the solutions[1] to the quantum constraint of the form

$$(\Psi| = (\Psi|^{(0)} + \varepsilon^2\,(\Psi|^{(2)}\ldots. \tag{5.7}$$

[1]We represent these solutions as generalized states; hence our notation as "bra" states.

At dominant order, the state is simply a solution of the FRW constraint, $(\Psi|^{(0)}\hat{\mathbf{C}}_0 = 0$. We discussed the form of the operator $\hat{\mathbf{C}}_0$ and the construction of solutions (starting from initial conditions at a minimum volume) in the previous section. If we go to the next perturbative order, we find that the evolution of the perturbations is dictated by the equation:

$$(\Psi|^{(2)}\hat{\mathbf{C}}_0 = -(\Psi|^{(0)}\left(\sum \hat{\mathbf{C}}_2^{\vec{n},\pm}\right)^{\dagger}, \tag{5.8}$$

where the dagger denotes the adjoint action. This equation can be solved exactly as the homogeneous FRW constraint, taking initial conditions on the section of minimum volume in the superselection sector and integrating in V, with a source given by the right hand side (and, therefore, by the quantum state at zeroth order). We thus see that the solutions are characterized again by their initial data at minimum volume. Consequently, we can identify quantum solutions with a space of initial conditions supplied with a Hilbert structure that ensures that the relevant observables become self-adjoint operators. In this way, e.g., we can choose the Hilbert space of physical states as $H_{kin}^{matt}\otimes\mathfrak{F}$ [16]. This concludes the quantization of our system.

6. Conclusion

We have studied a perturbed FRW universe with a massive scalar field. We have considered the case of compact flat spatial sections with the topology of a three-torus, and focused our discussion on scalar perturbations of the field and the space-time metric. In order to carry out our analysis of the quantization of this cosmological system within the framework of LQC, we have introduced two approximations. First, we have truncated the gravitational action at second order in the perturbations. Second, we have adopted a hybrid quantization scheme, which combines loop and Fock techniques, assuming that the most important quantum effects of the geometry are those that affect the FRW background. We have fixed the gauge of the linear perturbative constraints and reduced the system. We have shown that this system is endowed with a symplectic structure and a (global) Hamiltonian constraint at the considered truncation order, in contrast with recent claims to the contrary in the literature [17, 18] (for the sake of clarity, let us also remark that the system is already symplectic before reduction). This global Hamiltonian constraint includes backreaction effects in the sense that it contains both the contribution of the homogeneous part of the system and a term which is quadratic in the perturbations.

It is worth emphasizing that, for our formulation, no internal time is necessary. Under some controlled approximations, if a matter clock is available, one may reach an *effective* quantum field theory for the perturbations in an FRW background dressed with quantum corrections. We have discussed how this is possible if one adopts a Born-Oppenheimer approximation, splitting the dependence of the quantum states in a part for the FRW geometry and another part for the perturbations, and assuming that the latter part, in comparison to the former, has a negligible momentum conjugate to the zero mode of the scalar field, which is used as internal time. In the reached quantum field theory, the dynamics of the perturbations is unitary, thanks to the Fock representation and matter field scaling that we have chosen.

Finally, to make clear that the quantization that we have put forward does not rest on any specific choice of internal time, we have constructed physical states (which satisfy the global Hamiltonian constraint) using a perturbative scheme. We have shown that, in this construction, the physical

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states can be characterized by their initial data at the minimum volume of the FRW geometry (in the superselection sector where this geometry is quantized). This allows us to identify physical states with those data, and complete the quantization by endowing the space of such data with a Hilbert structure, determined, e.g., by requirements of self-adjointness on a complete set of observables.

The availability of a consistent quantization and of a space of physical states, as well as of approximations like the Born-Oppenheimer one, which lead to a quantum field theory for the perturbations in a background which is dressed with corrections from loop quantum geometry, places us in an adequate position to start analyzing effects of the quantization of gravity in the primordial fluctuations. The modifications to the Mukhanov-Sasaki equation that result from this quantum formalism may have left imprints in the cosmic radiation. The investigation of such imprints and the feasibility of their observation are issues that we are presently considering.

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