Towards a reduced phase space quantization in loop quantum cosmology with an inflationary potential

Kristina Giesel\textsuperscript{1}, Bao-Fei Li \textsuperscript{2} and Parampreet Singh\textsuperscript{2}\textsuperscript{†}

\textsuperscript{1} Institute for Quantum Gravity, Department of Physics, FAU Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen, Germany
\textsuperscript{2} Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803, USA

We explore a reduced phase space quantization of loop quantum cosmology (LQC) with Gaussian and Brown-Kuchař dust, and massless Klein-Gordon scalar reference fields for a spatially flat FLRW model with a Starobinsky inflationary potential. This is a “two-fluid” model in which reference fields act as global clocks providing a physical time in an inflationary spacetime, and allow bypassing various technical hurdles in conventional quantum cosmological models. The reduced phase space is obtained in terms of the Dirac observables of the gravitational as well as the inflaton degrees of freedom. The physical Hamiltonians of the two dust models take the same form but turn out to be quite different from that of the Klein-Gordon reference field which reflects an aspect of the multiple choice problem of time. Loop quantization is implemented using the so-called $\bar{\mu}$ scheme and the Schrödinger equations involving the physical Hamiltonian operators generating the evolution in the physical time in the dust and massless Klein-Gordon models are obtained. These turn out to be quantum difference equations with same non-singular structure as for other models in LQC. We study some phenomenological implications of the quantization using the effective dynamics resulting from the reduced phase space quantization including the resolution of the big bang singularity via a quantum bounce, and effects of the different reference fields on e-foldings in both the pre-inflation and the slow-roll inflationary phases. We find that different clocks, even when starting with a small but same energy density, can leave tiny but different imprints on the inflationary dynamics. In addition, for Brown-Kuchař dust, the choice of a negative energy density can result in a cyclic evolution before the onset of inflation constraining certain values for ideal clocks.

I. INTRODUCTION

In canonical quantum gravity a challenging question is associated with how to consistently extract a physical evolution. For general relativity (GR), the Hamiltonian is a linear combination of the first class constraints, and identically vanishes in the physical sector defined by the constraint hypersurface. As a result, the Hamiltonian is a gauge generator of spacetime diffeomorphisms and the generated ‘time evolution’ is not the true physical evolution as understood for the case of systems which are not totally constrained as GR. This leads to the fundamental problem of time in canonical gravity which must be successfully resolved to obtain any consistent dynamical evolution. The problem of time in canonical quantum gravity is complex and comes in different forms, which include the existence of a global time, and the multiple choice problem \cite{1}. Since these issues affect the way one interprets predictions from quantum gravity and quantum cosmology, they are necessary to be squarely addressed to obtain a consistent dynamics and phenomenology. In the quantization of GR as a totally constrained system, a related important issue which one encounters

\textsuperscript{*}Electronic address: kristina.giesel@gravity.fau.de
\textsuperscript{†}Electronic address: baofeili1@lsu.edu
\textsuperscript{‡}Electronic address: psingh@lsu.edu
is to find the physical Hilbert space equipped with a physical inner product. In general, this is a non-trivial task, such as in the Dirac’s method of the quantization of constrained systems where it requires a successful implementation of the refined algebraic quantization or the group averaging procedure [2]. In certain situations, which are of significant physical interest, all above issues need to be addressed together. One such situation arises in the presence of inflationary potentials where these issues become intricate, such as what is the choice of appropriate clocks, how to satisfy a global time requirement in inflationary dynamics and how it affects unitarity, and how to construct the associated conserved physical inner product.

Given that the inflationary paradigm is widely considered essential to explain cosmological observations, and since it is past-incomplete in classical GR, obtaining a quantization of inflationary spacetimes which is non-singular is an important open issue. The premise of our work deals exactly with such issues. For concreteness we choose the Starobinsky inflationary potential favored by observations and use techniques of loop quantum cosmology [3]. Our analysis can be extended easily to Wheeler-DeWitt quantum cosmology as well as other potentials, including those used as alternatives to inflation. Though our work uses established techniques in LQC, it is based on a reduced phase space quantization unlike the Dirac quantization which has been mainly used to study the quantization of various spacetimes in LQC so far.

To overcome the problem of time in quantum gravity, a strategy followed was to formulate dynamics in a relational way which was first studied by Bergmann, Komar [4-6] and further investigated by Kuchař and Isham [7], and more recently by Anderson [8]. A conceptual improvement by introducing the relational formalism was obtained by Rovelli [9, 10], further developed by Vytheeswaran [11], and mathematically further improved and analyzed by Dittrich [12, 13] and Thiemann [14] as well as by Pons, Salisbury and Sundermeyer [15, 16]. The idea of the relational formalism is to introduce reference fields with respect to which the dynamics of the remaining degrees of freedom is formulated. In the relational formalism, the observables can be constructed from phase space functions via an observable map introduced in [11, 12]. The resulting gauge-invariant quantities, so-called Dirac observables Poisson commute with all first class constraints. The relational formalism has been successfully used in various settings to extract dynamics in GR [13, 17-25], scalar-tensor theories [26], Lemaître-Tolman-Bondi spacetimes [27], loop quantum gravity (LQG) [28, 36] and quantum cosmological models [37-48]. The latter provide a simpler setting where the Gauss and spatial-diffeomorphisms are fixed in a symmetry reduction, and a single massless scalar field is most widely used as a reference field both in the Wheeler-DeWitt quantum cosmology [37, 38] and LQC [39-42].

Relational dynamics in LQC is mostly used in Dirac quantization where physical solutions are obtained by demanding the vanishing of the quantum Hamiltonian constraint, resulting in a quantum gravitational Klein-Gordon equation in isotropic models, which can be formulated as a Schrödinger equation after taking a square root. The resulting quantum evolution equation is a non-singular quantum difference equation with uniform steps in volume. The physical inner product can be obtained by a group averaging procedure or by demanding that the operators corresponding to the independent Dirac observables be self-adjoint [40]. This strategy, first set in place for LQC for a spatially flat isotropic and homogeneous Friedmann-Lemaître-Robertson-Walker (FLRW) model [40-42], has been successfully demonstrated for various spacetimes including those with spatial curvature [43, 44], a cosmological constant [41, 45-47] and radiation [48]. Dirac observables, such as the ones corresponding to the volume of the universe and the energy density of the matter content, constructed from using a massless scalar field relational clock are used to understand the resolution of singularities. At the quantum level, expectation values of these Dirac observables show that the big bang singularity is resolved via a quantum bounce occurring when the spacetime curvature reaches Planckian values. Using consistent histories formulation, probability for bounce to occur turns out to be unity [49]. Based on these results various extensions have
been successfully pursued, including investigations on a generic resolution of singularities \cite{50, 51}, quantization of anisotropic models \cite{52}, inclusion of inhomogeneities in Gowdy models \cite{53, 54}, and various phenomenological implications have been studied (see \cite{55} for a review). Despite this remarkable success, it is difficult to adopt above strategy to inflationary spacetimes because of a resulting time-dependent Hamiltonian constraint if one employs a single scalar field as is usually done in LQC, which in this case is the inflaton, as the clock. This complicates the task of finding the physical Hilbert space equipped with a conserved inner product in the time-dependent case. In cosmological models one may be tempted to choose a geometric time such as the scale factor or volume as an alternative. But apart from the Hamiltonian being still time-dependent, such a choice is also problematic in LQC due to the non-monotonicity of the scale factor because of the bounce. Further, using the momentum of the scale factor as a clock is also difficult to apply in loop quantization \cite{56}, making the implementation of geometric time in LQC challenging. Notably, in the case if the effect of the potential is small in the pre-inflationary epoch, one can consider a local time range in which the inflaton clock behaves monotonically and one finds that the big bang singularity is resolved \cite{57}. While such an approach does not provide a full quantum gravitational treatment of an inflationary spacetime where above issues are resolved, it does allow to gain some insights on the physics of bounce if potential plays little role \cite{57} and associated phenomenology \cite{58}, which has proved useful to get glimpses of quantum gravity effects via cosmological perturbations (see for eg. \cite{55, 59, 60}).

An alternative strategy to Dirac quantization is the reduced phase space quantization, where one again starts with choosing appropriate clocks, but reduces the constraints already at the classical level by constructing Dirac observables for just the remaining degrees of freedom which form the phase space variables of the reduced phase space. The physical Hamiltonian being a function of these Dirac observables in the reduced phase space is proportional to the momentum of the clock and is a constant of motion in the FLRW models considered here. Depending on the choice of the reference fields, the physical Hamiltonian can take different forms. So far, the reference fields have been mainly taken to be either dust reference fields or Klein-Gordon scalar fields (see \cite{20} and references therein). Although the additional scalar and dust degrees of freedom are introduced, for the dust and scalar field models the total Hamiltonian constraint of the resulting system can be easily cast into a form which is linear in the clock momentum and allows a simple derivation of the physical Hamiltonian. After quantization, this physical Hamiltonian directly results in an evolution operator for the quantum dynamics via a quantum gravitational Schrödinger equation. Unlike Dirac quantization, models with reference fields open the possibility to reduce part of the constraints or all of them at the classical level and then either part of or all the constraints are already taken care of before quantization. Two most common choices in the literature in the case of GR are that one considers four reference fields, one for the Hamiltonian constraint and three further ones associated with the spatial diffeomorphism constraint, or models with just one reference field for the Hamiltonian constraint. In \cite{20} these two kinds of models have been classified as models of type I and type II respectively. If one proceeds towards a quantization of these models the main difference of type I and type II manifests in the fact that for models of type I a quantization of the reduced phase space yields directly the physical Hilbert space\footnote{If one applies a loop quantization to the reduced phase space one has in addition to the Hamiltonian and spatial diffeomorphism constraint also the Gauss constraint, which in all of these models can be easily solved in the quantum theory.}, whereas in models of type II the spatial diffeomorphism constraints are handled via Dirac quantization which requires one to work in the diffeomorphism invariant Hilbert space in the case of full LQG as for instance done in \cite{29} or the model in \cite{31} where the quantization is performed in the algebraic quantum gravity framework \cite{61}.
In this work we will focus on models of type I which allow to derive the reduced phase space in terms of Dirac observables, where the latter can be explicitly constructed in the relational formalism once the reference fields have been chosen. Then from a quantization of the reduced phase space we directly obtain the physical Hilbert space by finding representations of the algebra of Dirac observables that in addition allow to implement the physical Hamiltonian as an operator on the physical Hilbert space. This step brings quantum gravity and quantum cosmology respectively in a situation usually given for unconstrained theories with a physical Hamiltonian operator that is not required to vanish in the physical Hilbert space. Given this one can then look for solutions of the obtained Schrödinger equation in above setting but unlike Dirac quantization this happens already at the level of the physical Hilbert space. Although these steps can be performed at the level of full GR yielding different models for LQG, the comparison of these different models in the framework of full LQG is a non-trivial task due to the far more involved mathematical structure of the full theory. Nevertheless it is an important question to understand different physical properties of these already existing models to see if there are any differences in physical predictions and understand the characteristic features of the individual models. An interesting analysis at the level of full LQG for two quantum gravity models of type II using perturbation theory for the physical Hamiltonian can be found [62].

In this article, we restrict our discussion to three different type I models and consider as a simpler case their symmetry reduction to a spatially flat FLRW universe with an inflationary potential where the inflaton is not chosen as a reference field (as in [57, 60]), but reference fields are coupled in addition to the inflaton. The latter has the advantage that the resulting physical Hamiltonian will be time-independent, whereas this is no longer the case when the inflaton is chosen as the clock with a non-trivial potential. Models of type I that can be considered in this context are for instance the Gaussian dust [20, 63], the Brown-Kuchař dust [18, 28, 64] and the four scalar field model [32, 33], where the latter in this work here has been extended by the coupling of an inflaton field which can be easily included into the constraint analysis. A model of type II that also provides a time-independent physical Hamiltonian even if the inflaton potential is considered is the one in [30, 31]. Similar to the four scalar field model [32, 33], the type II model in [29], although not analyzed in this direction so far, could also be generalized to more degrees of freedom including an inflaton coupled in addition to the reference field but for the model in [29] this needs to be implemented at the level of the diffeomorphism invariant Hilbert space and it would be interesting to compare such a generalizations to the generalized model of [32, 33]. An important point to mention here is that in the case of the background FLRW cosmology, the difference between models of type I and type II is absent due to the fact that the diffeos are trivially vanishing and hence in a symmetry reduced FLRW model only one reference fields is needed anyway. So for instance in the case of homogeneous FLRW cosmologies, the model [29] and the model [32, 33] both coincide and can be both understood as equally well justified generalizations of the LQC model in [39, 41]. Similarly, the Gaussian dust model, the Brown-Kuchař dust model as well as the model in [30, 31] all merge into the same model if we go to the symmetry reduced sector of FLRW\(^2\). However, if we go beyond the background dynamics and consider perturbations, which is an important arena to explore to connect quantum gravity effects with observations, the distinction between type I and type II models becomes quite relevant and in general we expect that all these models leave a different imprint in a cosmological perturbation analysis. In addition, even within one class of models, multiple choices of time can lead to different physical predictions. Hints of such potential differences were seen at the level of choosing different reference fields in type I models.

\(^2\) Here we assumed that certain sign choices have been fixed at the classical level, see the discussion in [20] for specific limits of the Brown-Kuchař model.
in the classical theory \cite{65}, and are discussed briefly later in the context of inflationary e-foldings. Moreover, since models of type II solve part of the constraint via Dirac quantization, whereas models of type I implement this by introducing three additional reference fields that backreact onto the system, a comparison of physical properties of models of type I and type II will also shed new light on the comparison between Dirac and reduced quantization, an important questions for LQG, and canonical quantum gravity in general. In this sense progress towards understanding the characteristic physical features of either models of type I or II is beneficial also for the other class of models.

A crucial first step towards perturbations around a quantum background spacetime with inflationary potentials is to understand and have full control of the symmetry reduced quantum FLRW model for which our analysis aims to provide a platform. In recent years, perturbations have been analyzed using the relational formalism in Dirac quantization in LQC with inflationary potentials via two main approaches \cite{58,60} (see also \cite{55} and references therein). In these studies, the inflaton is considered as a clock which due to limitations mentioned earlier does not permit a faithful treatment of quantum gravitational inflationary spacetimes and one is restricted to phenomenologically understand cases where the potential plays a little role. To understand the physical Hilbert space, physical inner product and physical solutions, one needs a different measure of time than one that has been chosen in various studies. One goal of this paper is to fill this gap and set a stage for understanding quantum gravitational inflationary spacetimes with consistent reference fields. Since in the models analyzed in this article the reference field is coupled in addition to the inflaton, one cannot just carry over the already existing techniques for perturbations around a quantum background spacetime, because these are so far restricted to the one-fluid case. Therefore, we need to go one step back and investigate the quantum background spacetime of the two-fluid models in detail before perturbations can be considered. The models that will be considered here have the common property that the algebra of the Dirac observables has the standard canonical form, which in general need not be the case. This is an important advantage as far as the reduced phase space quantization is concerned because in this case we can use the standard LQC representation, usually used for the kinematical Hilbert space in a Dirac quantization approach, as the representation for the physical Hilbert space here generalized to the case of two-fluid models. This is in contrast to the Dirac quantization, where obtaining the physical Hilbert space is non-trivial and involves finding inner product using group averaging procedure.

The main goal of this manuscript is to explore a reduced phase space quantization of LQC with Gaussian, Brown-Kuchař dust fields and a massless Klein-Gordon reference field. We consider a spatially flat FLRW universe sourced with an inflationary potential, taken to be the Starobinsky potential. Investigations of inflationary potentials, including the Starobinsky potential have been undertaken earlier in LQC but neither there is any study so far at the full quantum level where the physical Hilbert space equipped with a physical inner product is known, nor there are investigations with clocks in addition to the inflaton. The classical physical Hamiltonian for the Gaussian and Brown-Kuchař dust models in this spacetime with a Starobinsky potential has been studied recently in \cite{65}. It turns out that due to the homogeneity and the isotropy of the spacetime, the background evolution of the universe obeys the same equations of motion in both dust models for the classical theory. It was found that the difference between the two models shows up only when linear perturbations around a FLRW spacetime are considered. The Friedmann and Raychaudhuri equations in the reduced phase space of the two dust models take the same form as in the classical theory while a fingerprint of the dust fields appears as an additional dust contribution to the total energy density and leaves different imprints in Mukhanov-Sasaki variable. Although introducing the dust reference fields avoids the problem of time in GR, the big bang singularity in the cosmological setting still remains. Further, if the energy density is negative and large, as it is possible for the Brown-Kuchař model, the universe can also face a future big crunch singularity after the recollapse
of the scale factor. As we would see these singularities are found to be resolved in the reduced phase space quantization presented in our analysis.

Interestingly, due to the property of the observable map that the observable of a function of the elementary phase space variables is just the function of the corresponding Dirac observables, the reduced phase space quantization of LQC shares many features of the polymer quantization in standard LQC. For example, in LQC, the polymer quantization uses the holonomies of the connection and the triads as the fundamental variables for quantization. Similarly, in the reduced phase space of the Gaussian, Brown-Kuchař dust models and the massless Klein-Gordon scalar field model, one can easily construct the Dirac observables corresponding to holonomies and the triads. The physical Hamiltonian can then be expressed in terms of these Dirac observables in the same way as it is done for the Hamiltonian constraint in terms of holonomies and triads in LQC. One difference is that here we have more degrees of freedom due to the fact that we couple the reference fields in addition to the inflaton and thus obtain two-fluid cosmological models. However, the main difference from LQC lies in the fact that, after quantization using a reduced phase space quantization we directly obtain the physical Hilbert space. The quantum dynamics of the physical states is then governed by a Schrödinger equation involving the physical Hamiltonian operator and the quantum evolution is obtained with respect to either the dust or the massless Klein-Gordon scalar field clocks. This is in contrast to studies in standard LQC conducted so far, where one uses the inflaton itself as a clock and the understanding of the physical Hilbert space of a time-dependent quantum constraint is rather complicated. The inner product used for models with a massless scalar field which have a time-independent quantum constraint is no longer valid in presence of inflationary spacetimes. This problem is overcome in our analysis where the dust and the massless Klein-Gordon scalar field clocks are coupled in addition to the inflaton and are therefore independent of the inflationary potential. The quantization procedure results in a time-independent non-singular physical Hamiltonian. The evolution of the quantum states is prescribed by the above mentioned Schrödinger equation which turns out to be a non-singular quantum difference equation.

As is often done in LQC, we assume the existence of an effective spacetime description incorporating modifications from the polymer quantization. Note that in our work, effective dynamics is assumed to be valid for multi-fluid systems including the reference fields and is used to study phenomenological consequences of different choices of clocks for inflationary spacetimes. We discuss the way how the fingerprints of the chosen clocks in terms of their energy densities involved in the dynamics affect the phases of pre-inflation and slow-roll inflation. We find that as long as the dust fields do not alter the qualitative dynamics of the background spacetime, such that inflation does not occur, both positive and negative energy densities leave some impact on inflationary e-foldings. While this impact can be easily reduced by appropriately choosing smaller initial energy densities of reference fields, different reference fields leave distinct traces in inflationary dynamics. In particular, we find that starting with the same initial conditions for the energy density of reference fields and other variables, the number of the pre-inflationary and the inflationary e-foldings in the dust models turn out to be different from those in the Klein-Gordon scalar field model. For a larger magnitude of negative energy densities, there appears a cyclic universe before inflation can set in. Since such energy densities change qualitative dynamics in a significant way, they are constrained to be not corresponding to those of ideal clocks. We find that in general dust clocks with positive energy density and Klein-Gordon field clock allow a sufficiently long phase of inflation which in the backward evolution is non-singular due to non-perturbative loop quantum effects. For dust clocks with negative energy density, there exist initial conditions where non-singular inflationary phase sets in with or without multiple cycles of contraction and expansion of the universe.

This paper is organized as follows. In Sec. [II] we give a brief review of the relational formalism using the Gaussian and Brown-Kuchař dust models as well as the Klein-Gordon scalar field model
in GR. The reduced phase space constructed from the observable map in these models is discussed in a concise way and the physical Hamiltonian will be given in each case. In order to analyze these models in the context of cosmology, we also explicitly discuss the symmetry reduced case of spatially flat FLRW spacetime with the resulting physical Hamiltonians. This will be taken as the starting point for the loop quantization of the spatially flat universe in the reduced phase space in Sec. III. For the latter purpose the reduced phase space of the flat FLRW universe is formulated in terms of the Dirac observables corresponding to holonomies and the triads and the physical Hamiltonians in three reference field models are expressed in terms of these fundamental Dirac observables. The quantization is then carried out in the $\bar{\mu}$ scheme used in LQC. The resulting Schrödinger equations formulated at the level of the physical Hilbert space here turn out to be quantum difference equations with same structure as in conventional LQC and are non-singular. In order to facilitate a numerical analysis, we will also discuss the effective dynamics of the quantized background spacetime in the dust and Klein-Gordon scalar field models. In Sec. IV numerical solutions for some representative initial conditions will be discussed when the late-time inflation is driven by a single scalar field with a Starobinsky potential. The emphasis will be placed on how the energy density of the chosen clocks can leave traces in inflationary phases, as well as the different effects caused by a positive dust energy density and a negative one. Finally, in Sec. V we will summarize and discuss the main results of the paper.

In our paper, we will use $\hbar = c = 1$ while keeping Newton’s constant $G$ explicit in equations. For numerical studies, Newton’s constant is also set to unity. Greek letters are used to denote the 4-dimensional spacetime indices while the Latin letters $a, b, c...$ are for the indices of the tensors on the 3-dimensional hypersurface.

II. REVIEW OF RELATIONAL FORMALISM WITH DUST AND SCALAR REFERENCE FIELDS

The relational formalism originates from the observation that due to the diffeomorphism invariance in GR, the values of the metric and the matter field at any particular spacetime point bear no physical meaning. Since GR is a fully constrained system in which the gauge transformations are generated by the Hamiltonian and diffeomorphism constraints, one has to first construct the Dirac observables which at least weakly commute with all the first-class constraints and then extract physical predictions from the theory. In the relational formalism, these Dirac observables are constructed by means of reference fields, whose values at each coordinate point are encoded in a gauge fixing condition. The observable evaluated at physical coordinates of a given field returns the value of the field when the reference fields take those particular values fixed by the gauge condition. Although one can choose the reference fields from the geometric degrees of freedom \[22-24\], it is often more convenient to consider dust or scalar fields as the reference fields \[18\ \[27\ \[56\] since the resulting physical Hamiltonian that generates the dynamics on the reduced phase space is time independent for these models. Furthermore, these dust and scalar field models have the property that the Poisson algebra of the observables satisfies the standard canonical commutation relation, which is not given in the case of geometric clocks. In this section, we will review the relational formalism for three choices of matter reference fields. We consider both the Gaussian and Brown-Kuchař dust reference fields as well as the four scalar field model presented in \[32\ \[33\]. As the content in this section has been extensively studied in the vast literature \[1\ \[3\ \[6\ \[9\ \[14\ \[18\ \[20\ \[22\ \[23\ \[25\ \[26\ \[67\], we will only go through the basic ideas and quote the main results. The ultimate purpose of Sec. II is to discuss the explicit form of the physical Hamiltonians in the reduced phase space in the relational formalism when Gaussian, Brown-Kuchař dust or four scalar fields are chosen as reference fields and when in addition the background spacetime is a spatially flat FLRW.
universe. This reduced phase space whose elementary variables are the Dirac observables together
with their dynamics encoded in the physical Hamiltonian will serve as the starting point for the
loop quantization of the spatially flat FLRW universe in the relational formalism in next section.

II.A. The relational formalism with Gaussian and Brown-Kuchař dust and scalar reference
fields

All three models considered in this section have the property that they lead to addition of matter
fields to GR coupled to a generic scalar field $\varphi$. In the case of the Gaussian and Brown-Kuchař
dust models these are 8 additional fields whereas in the case of four scalar field model these are
7 additional fields. All systems are second class systems and the partial reduction of the second
class constraints in the individual models leads to a first class system with four additional reference
fields. In addition to gravity we consider a generic scalar field $\varphi$ and in the case of the dust models
8 fields denoted by $T^\mu = (T, S^j, \rho, W_j)$ where $j = 1, 2, 3$ on a four-dimensional hyperbolic spacetime
$(\mathcal{M}, g)$. In the case of the scalar field model we denote the additional scalar fields by $(\chi^0, \chi^j, M_{jj})$
where again $j = 1, 2, 3$. The total action of the coupled system is given by

$$S = S_{\text{geo}} + S_{\text{scalar}} + S_{\text{ref}},$$

where the first two terms of the action are given respectively by

$$S_{\text{geo}} = \frac{1}{2\kappa} \int_{\mathcal{M}} d^4x \sqrt{-g} R^{(4)},$$

$$S_{\text{scalar}} = \frac{1}{\lambda_\varphi} \int_{\mathcal{M}} d^4x \sqrt{-g} \left( -\frac{1}{2} g^{\mu\nu} \partial_\mu \varphi \partial_\nu \varphi - U(\varphi) \right),$$

with $\kappa = 8\pi G$, $R^{(4)}$ denotes the four-dimensional Ricci scalar, $\lambda_\varphi$ is a coupling constant allowing
for a dimensionless $\varphi$ and $U(\varphi)$ is the scalar potential. The last term $S_{\text{ref}}$ in action (2.1) depends
on the reference field model under consideration. In the Gaussian dust model, the dust action is
given by

$$S_{\text{ref}} = S^G_{\text{dust}} = -\int d^3x \sqrt{-g} \left( \frac{\rho}{2} [g^{\mu\nu} T_\mu T_\nu + 1] + g^{\mu\nu} T_\mu W_j S^j_\nu \right),$$

while in the Brown-Kuchař dust model, the dust action is given by

$$S_{\text{ref}} = S^{\text{BK}}_{\text{dust}} = -\frac{1}{2} \int_{\mathcal{M}} d^4x \sqrt{-\rho g} [g^{\mu\nu} \tilde{U}_\mu \tilde{U}_\nu + 1],$$

with the unit time-like dust velocity field defined by $\tilde{U} = -dT + W_j dS^j$, where $j = 1, 2, 3$. For the
scalar field model the action reads

$$S_{\text{ref}} = S^\text{ref}_{\text{scalar}} = -\frac{1}{2} \int_{\mathcal{M}} d^4x \sqrt{-g} g^{\mu\nu} \chi_\mu^0 \chi^0_\nu - \frac{1}{2} \int_{\mathcal{M}} d^4x \sqrt{-g} g^{\mu\nu} M_{jj} \chi^j_\mu \chi^j_\nu,$$

where the main motivation for introducing only seven but not add additional scalar fields in the
last model comes from the aim to formulate a model close to the model in [29] where only one
Klein-Gordon scalar field was taken as the temporal reference field but none for the spatial diffeo-
morphisms. In this way we choose the same temporal reference field as in [29]. As shown in [32]
considering a model with only four Klein-Gordon scalar fields as reference fields yields a physical
Hamiltonian that cannot be quantized in the framework of LQG.
Let us briefly summarize the main properties of the different models. In both of the Gaussian and Brown-Kuchař models, the dust field action involves eight scalar degrees of freedom, collectively denoted by $T^\mu = (T, S^j)$ and $(\rho, W_j)$. For both models adding the dust action to gravity plus standard matter yields a second class system. If we introduce the corresponding Dirac bracket the second class constraints can be solved strongly. In the partially reduced system the four dust fields $T^\mu = (T, S^j)$ are dynamical, whereas the scalar fields $(\rho, W_j)$ can be expressed in terms of the remaining variables in the partially reduced phase space. For the variables on the partially reduced phase space the Dirac bracket coincides with the Poisson bracket. The detailed analysis of the Hamiltonian formulation of the dust models [18, 20] reveals that, although in the extended phase space, there are 38 local degrees of freedom which include lapse $N$, shift $N^a$, 3-metric $q_{ab}$, the scalar field $\varphi$, the dust fields $T^\mu = (T, S^j)$, $(\rho, W_j)$ and their respective conjugate momenta, there are also 8 first class constraints and 8 second class constraints which result in a total of 14 physical degrees of freedom in the finally reduced phase space also called physical phase space. In the partially reduced phase space in which only the second class constraints have been implemented the elementary variables are the variables $N, N^a, q_{ab}, \varphi$ and $T^\mu$ and their conjugate momenta and 8 first class constraints. These first class constraints consist of four primary constraints and four secondary constraints. The primary constraints are the conjugate momenta of the lapse function and shift vector, i.e. $\pi_\mu = (\pi, \pi_a)$. The secondary constraints are the total Hamiltonian and spatially diffeomorphism constraint which take different forms in two dust models that will be discussed separately in the following. Going from the partially reduced phase space to the physical phase space can be achieved by applying the observable map to all elementary variables on the partially reduced extended phase space. The independent physical degrees of freedom are encoded into the Dirac observables of the variables $(q_{ab}, p^{ab})$ and $(\varphi, \pi_\varphi)$, which in this model can also be identified with the physical degrees of freedom.

In the scalar field reference model we start with seven additional scalar fields $(\chi^0, \chi^j, M_{jj})$ next to gravity and a scalar field with potential, so in total with 36 degrees of freedom in phase space. Again the resulting system is second class and the 6 second class constraints can be used to eliminate the $M_{jj}$ and their conjugate momenta. In this partially reduced phase space we have 30 degrees of freedom consisting of $N, N^a, q_{ab}, \varphi, \chi^0, \chi^j$ and their conjugate momenta together with 8 first class constraints. The latter include the primary constraints, that is the vanishing of the momenta for lapse and shift, as well as the secondary ones, being the Hamiltonian and spatial diffeomorphism constraints which here involve the corresponding contributions from the scalar reference fields. Now we can proceed as in the dust models and use $\chi^0, \chi^j$ as reference fields and construct Dirac observables. The reduced phase space in this model consists of the Dirac observables associated with $(q_{ab}, p^{ab})$ and $(\varphi, \pi_\varphi)$, which in this model can also be identified with the physical degrees of freedom.

In the following three subsections we briefly present the formulas and properties of the individual models that are relevant for our work in this article.

II.A.1. The Gaussian dust field model

In the Gaussian dust model, after the partial reduction of the second class constraints, the Hamiltonian and spatial diffeomorphism constraints, which are collectively denoted by $c^\mu_{\text{tot}} = \ldots$
\( (c^\text{tot}, c^\text{tot}_j) \), are of the form

\[
c^\text{tot} = P_T + c\sqrt{1 + q^{ab}T_{a,b} - q^{ab}T_{a}c_b} =: P_T + h^G,
\]
\[
c^\text{tot}_j = P_j + S^a_j \left(-h^G T_{a} + c_a \right),
\]

where \( P_T \) and \( P_j \) are conjugate momenta of \( T \) and \( S^j \). \( S^j \) is the inverse of \( S^a_i \) with \( S^a_a S^a_b = \delta^a_b \) and \( S^a_j S^j_b = \delta^a_b \). Further, \( h^G \) is defined by \( h^G := c\sqrt{1 + q^{ab}T_{a,b} - q^{ab}T_{a}c_b} \) with \( c \) and \( c_a \) given by

\[
c = \frac{1}{\sqrt{q}} \left( p_{ab}p^{ab} - \frac{1}{2} (p^{ab}q_{ab})^2 \right) - \sqrt{q} R^{(3)} + \frac{\kappa \lambda \varphi}{\sqrt{q}} \pi^2 + \frac{2 \kappa \sqrt{q}}{\lambda \varphi} \left( \frac{1}{2} q^{ab} \partial_a \varphi \partial_b \varphi + U \right),
\]
\[
c_a = -2q_{ab}D_c p^{bc} + 2\kappa \pi \partial_a \varphi,
\]

where \( p^{ab} \) and \( \pi_\varphi \) are the conjugate momenta of \( q_{ab} \) and \( \varphi \), respectively, and \( q \) is the determinant of the 3-metric. Next let us introduce the notation to collectively denote the secondary and primary constraints \( c_I = (c^\text{tot}_I, \pi_\mu) \) and reference fields and their temporal derivatives \( T^I = (T^\mu, \dot{T}^\mu) \) with the multi-index \( I = 1, \ldots, 8 \). In order that the reference fields can be used to construct Dirac observables, an important condition they need to satisfy is that \( T^I \) and \( c_J \) form a canonical conjugate pair, that is,

\[
\{ T^I (t, \vec{x}), c_J (t, \vec{y}) \} \approx 2\kappa \delta^I_J \delta (\vec{x} - \vec{y}).
\]

which is satisfied for both dust models. The corresponding gauge fixing conditions for the reference fields are given by \( G^I = (G^\mu, \dot{G}^\tau) \) with \( G^\mu = \tau^\mu - \dot{T}^\mu \), where \( \tau^\mu = (\tau, \dot{\sigma}) \) are functions on \( \mathcal{M} \) but not dynamical variables on the phase space. With this, one can construct an observable map for an arbitrary function \( f \) on the (partially reduced with respect to the second class constraints) extended phase space, which maps \( f \) to its gauge-invariant extension \( \mathcal{O}_{f,T^\mu} \), that is \( f \mapsto \mathcal{O}_{f,T^\mu}(\tau^\mu) \) and performs a reduction with respect to the remaining first class constraints. The explicit form of this map is given by

\[
\mathcal{O}_{f,T^\mu}(\tau^\mu) = f + \sum_{n=1}^{\infty} \frac{1}{n! 2^n \kappa^n} \prod_{k=1}^{n} \int d^3 x_k G^J(x_k) \{ f(x), c_J(x_k) \}_{(n)},
\]

where \( \{ f, g \}_{(n)} \) denotes the iterated Poisson bracket with \( \{ f, g \}_{(0)} = f \) and \( \{ f, g \}_{(n)} = \{ \{ f, g \}_{(n-1)}, g \} \). As discussed in detail in [18], the construction of the observables is performed in two steps. First a reduction with respect to the spatially diffeomorphism constraints is obtained by means of pulling back all variables in the phase space except \( (S^j, P_j) \) to the dust manifold yielding spatially diffeomorphism invariant quantities. In the second step the observable map is applied to these variables to further obtain the reduction with respect to the Hamiltonian constraint and the primary constraints, where the latter has not been discussed in [18, 20], but the explicit form of lapse and shift has been obtained via an alternative route. The Dirac observable \( \mathcal{O}_{f,T}(\tau) \) is the image of \( f \) under the observable map. For each \( \tau^\mu \), it returns the value of \( f \) in the gauge in which the reference fields \( T^\mu \) take the values \( \tau^\mu \). It is also straightforward to show that \( \mathcal{O}_{f,T}(\tau) \) weakly Poisson commutes with all the constraints \( c_I \) by using the property in (2.11). The elementary canonical variables in the reduced phase space are made up of the Dirac observables of the 3-metric, the scalar field and their respective momenta. More specifically, to keep our notation compact, we use the notation for these elementary observables to simply denote them by the corresponding capital letters as

\[
Q_{ij} := \mathcal{O}_{q_{ij},T}[\tau, \dot{\sigma}], \quad P^{ij} := \mathcal{O}_{p^{ij},T}[\tau, \dot{\sigma}], \quad \Phi := \mathcal{O}_{\varphi,T}[\tau, \dot{\sigma}], \quad \Pi_\Phi := \mathcal{O}_{\pi_\varphi,T}[\tau, \dot{\sigma}].
\]
Meanwhile, from the observable map (2.12), one can find that in the Gaussian dust model
\[ O_{\pi_{\mu},T}[\tau, \vec{\sigma}] = \pi_{\mu}, \quad O_{T_{\mu},T}[\tau, \vec{\sigma}] = T_{\mu}. \]
Now for the particular choice of the gauge fixing condition
\[ G_{\mu} = \tau_{\mu} - T_{\mu}, \quad \text{with} \quad \tau_{\mu} = x_{\mu}. \]
the observable of the lapse function and the shift vector satisfy the Gaussian coordinate condition
\[ O_{N,T}[\tau, \vec{\sigma}] = 1, \quad O_{Nj,T}[\tau, \vec{\sigma}] = 0. \]
As a result, choosing Gaussian dust reference fields \( T_{\mu} \) yields Dirac observables for lapse and shift that correspond to a Gaussian reference frame. The physical Hamiltonian that generates the dynamics of the physical degrees of freedom, that is the independent degrees of freedom in the physical phase space is for the Gaussian dust model given by
\[
H_{\text{phys}}^G = \frac{1}{2\kappa} \int_S d^3\sigma \, O_{h_{\mu},T} = \frac{1}{2\kappa} \int_S d^3\sigma \, C, \quad C := O_{c,T}(Q^{ij}, P_{ij}, \Phi, \Pi_{\Phi}),
\]
where \( C \) is obtained from replacing each dynamical variable in (2.9) by their respective observables defined in (2.13), which can be shown by using the properties of the observable map. More specifically,
\[
C = \frac{1}{\sqrt{Q}} G_{ijmn} P^{ij} P^{mn} - \sqrt{Q} R^{(3)} + \frac{\kappa \lambda_{\varphi} \Pi_{\Phi}^2}{\sqrt{Q}} + \frac{2\kappa}{\lambda_{\varphi}} \left( \frac{1}{2} Q^{ij} \delta_{ij} \delta_{ij} + U \right),
\]
with
\[
G_{ijmn} = \frac{1}{2} (Q_{im} Q_{jn} + Q_{in} Q_{jm} - Q_{ij} Q_{mn}).
\]
With the fundamental Poisson brackets of the canonical variables in the reduced phase space given by,
\[
\{ Q_{ij}[\tau, \vec{\sigma}], P^{kl}[\tau, \vec{\sigma}'] \} = 2 \kappa \delta_{ij} \delta_{kl} \delta^{3}(\vec{\sigma} - \vec{\sigma}'),
\]
\[
\{ \Phi[\tau, \vec{\sigma}], \Pi_{\Phi}[\tau, \vec{\sigma}'] \} = \delta^{3}(\vec{\sigma} - \vec{\sigma}'),
\]
the dynamics of a generic function \( F \) on the reduced phase space is governed by Hamilton’s equations
\[
\dot{F} = \frac{dF}{d\tau} (Q_{ij}, P^{ij}, \Phi, \Pi_{\Phi}) = \{ F, H_{\text{phys}}^G \} = \frac{1}{2\kappa} \int_S d^3\sigma \{ F, C(\sigma) \}
\]
and this can be used to derive the equation of motion for the elementary Dirac observables.

II.A.2. The Brown-Kuchař dust reference model

If we perform a partial reduction with respect to the second class constraints in the Brown-Kuchař dust model, the Hamiltonian and spatial diffeomorphism constraints can be expressed as
\[
c_{\text{tot}} = P_T - \text{sgn}(P_T) \sqrt{c^2 - q^{ab}c_a c_b} =: P_T - \text{sgn}(P_T) h_{\text{BK}},
\]
\[
c_{ij} = P_j + S_j (\text{sgn}(P_T) h_{\text{BK}})^a c_a,
\]
where \( \text{sgn}(P_T) \) denotes the sign of \( P_T \) and \( h_{\text{BK}} := \sqrt{c^2 - q_{ab}c_a c_b} \). The details of the relational formalism with Brown-Kuchař dust fields can be found in [13]. Following the same line of argument as in the Gaussian dust case, the physical Hamiltonian is the observable associated with \( h_{\text{BK}} \), which yields

\[
H_{\text{phys}}^{\text{BK}} = \frac{1}{2\kappa} \int_S d^3\sigma \; O_{h_{\text{BK}},T} = \frac{1}{2\kappa} \int_S d^3\sigma \; \sqrt{c^2 - Q^{ij}C_i C_j} =: \frac{1}{2\kappa} \int_S d^3\sigma \; H(\sigma). \tag{2.24}
\]

Here \( H := \sqrt{c^2 - Q^{ij}C_i C_j} \) denotes the physical Hamiltonian density. \( C \) is given in (2.17) and \( C_i \) is the image of (2.10) under the observable map, which is explicitly given by

\[
C_i = -2D_k P^k_i + 2\kappa \Pi \Phi \partial_i \Phi. \tag{2.25}
\]

It should be noted that in order to obtain the Hamiltonian (2.24), we choose \( \text{sgn}(P_T) \) to be negative so that (2.24) is bounded from below. The application of the observable map in (2.12) to lapse and shift degrees of freedom leads for the Brown-Kuchař model to the following observables:

\[
\mathcal{O}_{N,T}(\tau, \vec{\sigma}) = \frac{C}{H} = \sqrt{1 + \frac{Q^{ij}C_i C_j}{H^2}}, \quad \mathcal{O}_{N_j,T}(\tau, \vec{\sigma}) = 0, \quad \mathcal{O}_{\pi,T}(\tau, \vec{\sigma}) = \pi, \quad \mathcal{O}_{\pi_j,T}(\tau, \vec{\sigma}) = \pi_j, \tag{2.26}
\]

which shows that in the Brown-Kuchař model, the lapse and shift degrees of freedom can be completely expressed in terms of the physical variables and the primary constraints. In [18, 19] a shift vector in terms of physical degrees of freedom is defined as \( N_j := -\frac{Q^{jk}C_k}{H} \) whereas above we present the Dirac observable associated to the shift vector which is just zero. Note that there is no contradiction between two results because the \( N_j \) from [18, 19] is not the Dirac observable of the shift vector but has been defined as follows. Consider \( \{F, H(\sigma)\} = \frac{C}{H} \{F, C\} - \frac{Q^{jk}C_k}{H} \{F, C_j\} \). Then \( N_j \) was defined as being the coefficient in front of the Poisson bracket of \( \{F, C_j\} \). The only non-vanishing Poisson brackets in the reduced phase space spanned by elementary canonical variables in (2.13) are still given by (2.19)-(2.20). As a result, the evolution of a generic phase space function \( F(Q_{ij}, P_{ij}, \Phi, \Pi_\Phi) \) is governed by Hamilton's equations

\[
\dot{F} = \{F, H_{\text{phys}}^{\text{BK}}\} = \int_S d^3\sigma \{F, H_{\text{phys}}^{\text{BK}}(\sigma)\}. \tag{2.27}
\]

that are generated by the physical Hamiltonian.

II.B. The four scalar field reference model

As for the former two models we discuss the form of the Hamiltonian and spatial diffeomorphism constraints after the second class constraints have been implemented. They take the following form:

\[
\epsilon^\text{tot} = p_{\chi^0} + h_{\text{scalar}}(q_{ab}, \pi^{ab}, \chi^0, \chi^j), \tag{2.28}
\]

\[
\epsilon^j_\text{tot} = p_{\chi^j} + \chi^j_a \left(-h_{\text{scalar}} \chi^0_a + c_a\right), \tag{2.29}
\]

with

\[
h_{\text{scalar}}(q_{ab}, \pi^{ab}, \chi^0, \chi^j) = -\frac{B}{2} - \sqrt{\left(\frac{B}{2}\right)^2 - A}, \tag{2.30}
\]
where

\[
B := -2\sqrt{q} \sum_{j=1}^{3} \chi_{a}^0 \varphi_{j} \sqrt{q^{cd} \chi_{c}^j \chi_{d}^j},
\]

\[
A := q q^{ab} \chi_{a}^0 \chi_{b}^0 - 2\sqrt{q} \sum_{j=1}^{3} \varphi_{j}^a c_{a} \sqrt{q^{cd} \chi_{b}^j \chi_{d}^j} + 2\sqrt{q} c .
\]

(2.31)

In this model we choose \( \chi^0 \) as the reference field for the Hamiltonian constraint and \( \chi^j \) as the ones associated with the spatial diffeomorphism constraint. Then one can proceed similarly to the dust models and construct Dirac observables given by

\[
Q_{ij} := O_{q_{ij}, \chi^0}[\tau, \vec{\sigma}], \quad P^{ij} := O_{p_{ij}, \chi^0}[\tau, \vec{\sigma}], \quad \Phi := O_{\phi, \chi^0}[\tau, \vec{\sigma}], \quad \Pi_{\Phi} := O_{\pi_{\phi}, \chi^0}[\tau, \vec{\sigma}],
\]

(2.32)

where as in the dust case to keep our notation compact we just use the temporal reference field as a label and in abuse of notation we denote the corresponding Dirac observables for all three models with the same capital since their meaning should be obvious from the context where they are applied.

The physical Hamiltonian that generates the dynamics of these observables on the reduced phase space has in the four scalar fields model the following form

\[
H_{\text{phys}} = \frac{1}{2\kappa} \int_{S} d^{3}\sigma O_{H_{\text{scalar}}, \chi^0} = \frac{1}{2\kappa} \int_{S} d^{3}\sigma \sqrt{-2\sqrt{Q} C + 2\sqrt{Q} \sum_{j=1}^{3} Q^{ij} C_j C_j^j}
\]

\[
= : \frac{1}{2\kappa} \int_{S} d^{3}\sigma H_{\text{scalar}}(\sigma),
\]

(2.33)

where \( C \) and \( C_j \) take the same form as in (2.17) and (2.25). A difference to the two dust models considered before is that here summation over \( j \) involved in the physical Hamiltonian density induces a kind of directional dependence at the level of the scalar field manifold for the reason that the \( C_j \)'s and the inverse metric \( Q^{jk} \) are not contracted in a covariant fashion. However, since this is at the level of the observables and refers to the scalar field manifold this causes no issue here. Moreover, in the context of this work where we consider the FLRW symmetry reduced case this term in the physical Hamiltonian will not contribute but vanishes in this sector. The reason for the form of this term can be understood once we look at the explicit form of the Dirac observables for lapse and shift and their conjugate momenta in this model. Those take the form

\[
O_{\chi^0, \chi^0}(\tau, \vec{\sigma}) = -\frac{\sqrt{Q}}{H_{\text{scalar}}}, \quad O_{\chi^j, \chi^0}(\tau, \vec{\sigma}) = \frac{\sqrt{Q} \sqrt{Q}^{ij}}{H_{\text{scalar}}}, \quad O_{\pi, \chi^0}(\tau, \vec{\sigma}) = \pi, \quad O_{\pi_j, \chi^0}(\tau, \vec{\sigma}) = \pi_j,
\]

(2.34)

As in the other two models the evolution of a generic phase space function \( F(Q_{ij}, P^{ij}, \Phi, \Pi_{\Phi}) \) on the reduced phase space is encoded in the Hamilton’s equations that are here given by

\[
\dot{F} = \{ F, H_{\text{phys}} \} = \int_{S} d^{3}\sigma \{ F, H_{\text{scalar}}(\sigma) \}
\]

(2.35)

from which the corresponding second-order equations of motion of the Lagrangian framework can be recovered.
II.C. The reduced phase space in a spatially flat FLRW universe

In this section we want to take the reduced phase spaces obtained in three models as a starting point and further symmetry reduce it to the case of a spatially flat FLRW universe. For the reason that we want to apply a reduced phase space quantization in the context of loop quantum cosmology later on we will consider the reduced phase spaces formulated in terms of Ashtekar-Barbero variables. If we perform the extension from the ADM phase space to the one where the Ashtekar-Barbero variables \((A^\mu_i, E_i^a)\) are the elementary ones we obtain an additional SU(2) Gauss constraint. This Gauss constraint will not be reduced by means of additional reference fields but can even within full LQG be solved via Dirac quantization at the quantum level. Hence, we can still consider models with four reference fields and because we go to the FLRW symmetry reduced sector the Gauss constraint plays anyway no role for our work presented here. Following the discussion of the former section we use in each of the presented models the reference fields and the observable map to obtain the Dirac observables of the (up to the Gauss constraint) reduced phase space that are for the two dust models denoted by

\[
\mathcal{O}_{A^\mu_i, T}[\tau, \vec{\sigma}], \quad \mathcal{O}_{E_i^a, T}[\tau, \vec{\sigma}], \quad \mathcal{O}_\varphi, T[\tau, \vec{\sigma}], \quad \mathcal{O}_{\pi, \varphi, T}[\tau, \vec{\sigma}],
\]

(2.36)

and in the case of the four scalar field model are given by

\[
\mathcal{O}_{A^\mu_i, \lambda^0}[\tau, \vec{\sigma}], \quad \mathcal{O}_{E_i^a, \lambda^0}[\tau, \vec{\sigma}], \quad \mathcal{O}_\varphi, \lambda^0[\tau, \vec{\sigma}], \quad \mathcal{O}_{\pi, \varphi, \lambda^0}[\tau, \vec{\sigma}].
\]

(2.37)

The corresponding physical Hamiltonians \(H_{\text{phys}}^G, H_{\text{phys}}^{\text{BK}}\) and \(H_{\text{phys}}^{\text{scalar}}\) are then understood as function of these Dirac observables.

If we specialize to the symmetry reduced FLRW sector we consider a spatially flat isotropic and homogeneous FLRW spacetime described by the metric

\[
ds^2 = -\mathcal{O}_N^2 d\tau^2 + Q_{jk} d\sigma^j d\sigma^k,
\]

(2.38)

respectively, where \(\tau\) is the physical time \(\tau\) of the dust models that can be interpreted as proper time and \(\tau_\chi\) denotes the physical time in the scalar field model, \(\mathcal{O}_N\) is the lapse function and \(Q_{jk}\) is the physical metric related to comoving coordinates as

\[
Q_{jk} d\sigma^j d\sigma^k = \mathcal{O}_{a^2} \hat{Q}_{jk} d\sigma^j d\sigma^k = \mathcal{O}_{a^2} ((d\sigma^1)^2 + (d\sigma^2)^2 + (d\sigma^3)^2).
\]

(2.39)

Here \(\hat{Q}_{jk}\) is the fiducial metric over the spatial manifold which for \(k = 0\) model can be \(\mathbb{R}^3\) or \(\mathbb{T}^3\). In the latter case, the scale factor \(a\) relates the coordinate volume \(V_{\hat{V}_0}\) of the 3-torus and the physical volume as \(\mathcal{O}_V = \mathcal{O}_{a^3 V_{\hat{V}_0}}\). If the spatial manifold is chosen with spatial topology \(\mathbb{R}^3\) then one needs to choose a fiducial cell (\(V\), acting as an infra-red regulator, to define symplectic structures. In this case, one is free to choose another cell which has a rescaled coordinate volume. A key requirement for consistency of physics in LQC is that physical predictions of observables which are classically invariant under rescalings of the fiducial cell must be invariant under such rescalings after quantization. It turns out that this requirement leads to so-called improved dynamics or the \(\mu\)-scheme as the only consistent quantization in isotropic LQC [68]. In our analysis we will focus on the \(\mu\)-scheme introduced in [31] in the next section.

Due to the homogeneity and isotropy of the spatially flat FLRW universe, the reduced phase space of the geometric sector is a two-dimensional space spanned by the canonical pair \((\mathcal{O}_c, \mathcal{O}_p)\) which are related with the Dirac observables of the Ashtekar-Barbero SU(2) connection \(\mathcal{O}_{A^\mu_i}\) and the densitized triad \(\mathcal{O}_{E_i^a}\) via

\[
\mathcal{O}_{A^\mu_i} = \mathcal{O}_c \mathcal{O}_{V_0^{-1/3}} \mathcal{O}_{\hat{q}_h^a}, \quad \mathcal{O}_{E_i^a} = \mathcal{O}_p \mathcal{O}_{V_0^{-2/3}} \sqrt{\hat{q}} \mathcal{O}\hat{\rho}_i^a,
\]

(2.40)
with $\mathcal{O}_{e_i}$ and $\mathcal{O}_{\omega_{ij}}$ representing the fiducial triads and co-triads compatible with the fiducial metric $\bar{Q}_{jk}$, respectively. The fiducial volume of $\mathcal{V}$ with respect to the fiducial metric $\bar{Q}_{jk}$ will be set to unity in the following. The canonically conjugate pair $(\mathcal{O}_c, \mathcal{O}_p)$ satisfies in all three models

$$\{\mathcal{O}_c, \mathcal{O}_p\} = 8\pi G \gamma/3$$

(2.41)

where $\gamma$ is the Barbero-Immirzi parameter in LQG whose value is conventionally set to $\gamma \approx 0.2375$ from black hole thermodynamics in LQG. Note that here and in the following the subscript $c$ in $\mathcal{O}_c$ denotes the symmetry reduced connection and does not correspond to the $c$ in (2.9) that denotes all but the reference contribution to the Hamiltonian constraint. Since we work in the reduced phase space, in the following the symmetry reduced connection is always depicted in its Dirac observable form and to avoid confusion the Dirac observable associated with $c$ from black hole thermodynamics in LQG. Note that here and in the following the subscript

$$\{\mathcal{O}_\phi, \mathcal{O}_\pi\} = 1,$$

(2.42)

where we again used the property that for the variables $\phi, \pi$ we have $\{\phi, \pi\}^* = \{\phi, \pi\}$. Now it remains to discuss the symmetry reduced form of the physical Hamiltonians for each of the models. In the case of the spatially flat FLRW spacetime, the observable $C_j$ in (2.25) vanishes and as a consequence the physical Hamiltonians in the Gaussian and the Brown-Kuchař dust model coincide which are the symmetry reduced version of the physical Hamiltonian given in (2.16). This fits well with the fact that in the case of spatially flat FLRW spacetime the Dirac observable of the lapse function $\mathcal{O}_{N,T}$ in (2.26) of the Brown-Kuchař model becomes unity and thus agrees with the corresponding Dirac observable of the Gaussian dust model. Since in the Brown-Kuchař dust model the physical Hamiltonian involves a square root, we briefly discuss this in a bit more in detail for this model. Considering the Hamiltonian constraint in (2.22), in the symmetry reduced case we obtain for the reduced phase space

$$P_T = \text{sgn}(P_T)\sqrt{C^2} = \text{sgn}(P_T)|C|$$

and the physical Hamiltonian will be given by $H_{\text{FLRW,dust}}^{\text{phys}} = -\text{sgn}(P_T)|C|$. Now from the original form of the constraints in the Brown-Kuchař dust model [18] we have $c^\text{tot} = c + P_T \sqrt{1 + g^{ab}U_a U_b}$, where $c$ is shown in (2.9) and this implies at the level of observables that on the constraint surface $\text{sgn}(c) = -\text{sgn}(P_T)$ from which we obtain $\text{sgn}(C) = -\text{sgn}(P_T)$. Considering this let us discuss the two possible cases: if the dust energy is negative, that is $P_T < 0$, then we have $H_{\text{FLRW,dust}}^{\text{phys}} = |C| = C$ where we used in the last step that for $P_T < 0$ we have $C > 0$. If the dust energy density is chosen to be positive, that is $P_T > 0$ we have $C < 0$ and thus $H_{\text{FLRW,dust}}^{\text{phys}} = -|C| = C$ in this part of the phase space. Thus we fix the sign of $C$ at the classical level and then quantize the corresponding sectors of the reduced phase space. As discussed in [20] this can become problematic since it requires to have sufficient control on the spectrum of the physical Hamiltonian which for full LQG is perhaps a too strong requirement. However, in the mini-superspace models considered here we assume that this assumptions is justified.

In order to make the integral in (2.16) finite, one can first choose a fiducial cell with the volume $\mathcal{O}_{\nu_i}$ in the symmetry reduced dust manifold, then compute all the integrals within the fiducial cell. As mentioned earlier, we choose the volume of this cell to be unity. The physical Hamiltonian of the dust models in the classical theory can be written in terms of the Dirac observables for the
symmetry reduced variables as

$$H_{\text{phys}}^{\text{FLRW, dust}} = -\frac{3\mathcal{O}_p^2 \sqrt{\mathcal{O}_p}}{\kappa^2} + \frac{\lambda \phi}{\kappa^2} + \frac{\mathcal{O}_p^{3/2} U(\mathcal{O}_p)}{\lambda \phi}.$$  \hfill (2.43)

It should also be noted that $H_{\text{phys}}^{\text{FLRW, dust}}$ is the physical Hamiltonian in the reduced phase space so it does not vanish but is a constant of motion which is determined by the initial conditions of the system.

In the case of the scalar field reference model the symmetry reduction of the physical Hamiltonian leads to the following form

$$H_{\text{phys}}^{\text{FLRW, scalar}} = -\frac{3\mathcal{O}_p^2 \sqrt{\mathcal{O}_p}}{\kappa^2} + \frac{\lambda \phi}{\kappa^2} + \frac{\mathcal{O}_p^{3/2} U(\mathcal{O}_p)}{\lambda \phi}.$$  \hfill (2.44)

This setup will be taken as the starting point of the reduced phase space quantization of the symmetry reduced flat FLRW sector for the three models. We will discuss in detail how the loop quantization can be applied for each of this models and derive in the next section the corresponding quantum operators for the physical Hamiltonians of the dust and scalar field model.

Finally, let us briefly summarize what we have done in this section, which started with a brief review on the relational formalism with the Gaussian, Brown-Kuchař dust and four scalar reference fields. In each model, the reduced phase space was discussed from the extended ADM phase space via the observable map. The images of the 3-metric and the scalar field under the observable map are the Dirac observables that constitute the elementary canonical variables in the reduced phase space. The dynamics of these Dirac observables is governed by a physical Hamiltonian in the reduced phase space. In the case of a spatially flat FLRW universe, the reduced phase space is further symmetry reduced to a four-dimensional minisuperspace which we have expressed in the gravitational sector in terms of connection and triad variables. While in the minisuperspace the physical Hamiltonian assumes the same form in the Gaussian and the Brown-Kuchař dust models, in contrast, in the scalar field model the physical Hamiltonian has a different form.

## III. LOOP QUANTIZATION OF THE SPATIALLY FLAT UNIVERSE IN THE RELATIONAL FORMALISM

In this section, we apply loop quantization to the reduced phase space of the dust models and Klein-Gordon scalar field model for a spatially flat FLRW universe. Then, we will proceed with the effective description of quantum spacetime and find the resulting Hamilton’s equations and modified Friedmann equation from an effective Hamiltonian. Then we perform numerical analysis using Hamilton’s equations in the next section. Let us note that conventional LQC allows different factor orderings, such as [41, 42, 69]. While we present results following the construction in [41], which also guides our notation, our results can be generalized in a straightforward way to other factor orderings.

For the two dust as well as the scalar field reference models we consider the reduced phase space symmetry reduced to a spatially flat FLRW universe discussed in Sec. [12, 69] as the starting point for quantization. What we are aiming at is to find a representation of the algebra of Dirac observables for each individual model that further allows to implement the physical Hamiltonian of the models as a well defined operator. In this approach we directly obtain a representation of the physical Hilbert space. This is in contrast to the usual approach in LQC with a scalar field clock. There one deparameterizes the Hamiltonian constraint at the classical level and then
performs a Dirac quantization by promoting the classical constraint to a constraint operator on the kinematical Hilbert space. Considering then states that are annihilated by the constraint yields a set of functions on which the physical inner product can be defined (see for instance [40, 41]), and taking the completion with respect to the corresponding norm yields the physical Hilbert space in this route.

An advantage of all these models have is that the algebra of the elementary Dirac observables in the reduced phase space is as simple as the kinematical algebra because we have for the dust models as well as the for the scalar field model

\[
\{O_c, O_p\} = \frac{8\pi G\gamma}{3}, \quad \{O_\varphi, O_{\pi_\varphi}\} = 1,
\]

where we as before neglected the label of the clocks here that would be \(T\) for the dust models and \(\chi^0\) for the scalar model. Since we want to apply a loop quantization, instead of the connections \(O_c\) and triads \(O_p\), the canonical variables used for quantization are the holonomies of the connection along edges and the fluxes of the triads along 2-surfaces. These can be constructed from our Dirac observables \(O_c\) as follows:

\[
\mathcal{O}_{\mu} = \cos\left(\frac{\mu O_c}{2}\right) \mathbb{1} + 2\sin\left(\frac{\mu O_c}{2}\right) \tau_k,
\]

where \(\mathbb{1}\) represents a unit 2 \(\times\) 2 matrix and \(\tau_k = -i\sigma_k/2\) with \(\sigma_k\) denoting the Pauli spin matrices. To obtain the above equation we have used that the observable map is a homomorphism with respect to the groups of multiplication and addition, that is for any functions \(f(c, p, \varphi, \pi_\varphi)\), in the original kinematical phase space, the observable map has the property

\[
\mathcal{O}_f(c, p, \varphi, \pi_\varphi, T) = (\mathcal{O}_c, T, \mathcal{O}_p, T, \mathcal{O}_\varphi, T, \mathcal{O}_{\pi_\varphi}, T) \quad \text{and} \quad \mathcal{O}_f(c, p, \varphi, \pi_\varphi, \chi^0) = (\mathcal{O}_c, \chi^0, \mathcal{O}_p, \chi^0, \mathcal{O}_\varphi, \chi^0, \mathcal{O}_{\pi_\varphi}, \chi^0)
\]

in the two dust models and in the scalar field model respectively.

The flux of the triads along 2-surfaces in the spatially flat FLRW spacetime turns out to be proportional to \(O_p^3\). The elementary variables that are chosen instead of \(O_c, O_p\) in LQC are the pair \(N_\mu(O_c) = e^{i\mu O_c/2}\) and \(O_p\), where \(\mu \in \mathbb{R}\) that satisfy the algebra

\[
\{N_\mu(O_c), O_p\} = \frac{4\pi G\gamma \mu}{3} N_\mu(O_c)
\]

At the quantum level, the first task is to find a representation of the \(\star\)-algebra generated by the elementary variables of the gravitational and matter sector. However, since the algebra of the elementary variables on our reduced phase space coincides exactly with the one at the kinematical level of LQC we can use the representation usually describing the kinematical Hilbert space of LQC \(\mathcal{H}_{\text{kin}}\) here as a representation of the physical Hilbert space \(\mathcal{H}_{\text{phys}}\). This is in exact analogy to the model presented in [28, 32, 33] based on a reduced quantization of full LQG.

### III.A. Physical Hilbert space and Hamiltonian operator of the dust models

As far as the gravitational sector of the theory is considered thanks to the methods in LQG [71, 72], a unique representation for the symmetry reduced model can be identified [73, 74], which can be used for the physical Hilbert space for the reference field models in our work. In the case of the two dust models the physical Hilbert space is \(\mathcal{H}_{\text{phys,grav}} = L^2(\mathbb{R}_{\text{Bohr}}, d\mu_{\text{Bohr}})\) where \(\mathbb{R}_{\text{Bohr}}\) is

---

\(^3\) For an alternate quantization using gauge-covariant fluxes see [70].
the Bohr compactification of the real line with Haar measure $\mu_{\text{Bohr}}$. The sector of the inflaton is quantized in the usual Schrödinger representation with the Hilbert space $\mathcal{H}_{\text{phys,} \varphi} = L^2(\mathbb{R}, d\mathcal{O}_\varphi)$. The physical Hilbert space of the theory is then just given by the tensor product of the individual Hilbert spaces $\mathcal{H}_{\text{phys}} = \mathcal{H}_{\text{phys,grav}} \otimes \mathcal{H}_{\text{phys,} \varphi}$. We denote the elements of $\mathcal{H}_{\text{phys}}$ by $\Psi(\mathcal{O}_c, \mathcal{O}_\varphi) := \psi(\mathcal{O}_c) \otimes \psi(\mathcal{O}_\varphi)$. The inner product of $\mathcal{H}_{\text{phys}}$ is given by

$$
\langle \Psi, \bar{\Psi} \rangle_{\text{phys}} := \langle \psi, \bar{\psi} \rangle_{\text{grav}} \langle \psi, \bar{\psi} \rangle_{\varphi}
$$

with the inner product in the gravitational sector

$$
\langle \psi, \bar{\psi} \rangle_{\text{grav}} := \lim_{D \to \infty} \frac{1}{2D} \int_{-D}^{D} d\mathcal{O}_c \bar{\psi}(\mathcal{O}_c) \psi(\mathcal{O}_c)
$$

and for the matter part we use the standard Schrödinger inner product given by

$$
\langle \psi, \bar{\psi} \rangle_{\varphi} := \int_{-\infty}^{\infty} d\mathcal{O}_\varphi \bar{\psi}(\mathcal{O}_\varphi) \psi(\mathcal{O}_\varphi).
$$

If we choose some orthonormal basis in $\mathcal{H}_{\text{phys,} \varphi}$ that we denote by $\psi_n$ with $n \in \mathbb{N}$ then an orthonormal basis in $\mathcal{H}_{\text{phys}}$ is given by the set $\{N_\mu(\mathcal{O}_c) \otimes \psi_n\}_{\mu \in \mathbb{R}, n \in \mathbb{N}}$ since $\langle N_\mu(\mathcal{O}_c)|N_{\mu'}(\mathcal{O}_c)\rangle_{\text{grav}} = \delta_{\mu,\mu'}$ where $N_\mu(\mathcal{O}_c)$ are almost periodic functions of $\mathcal{O}_c$. Normalizable quantum states are given by a tensor product of a discrete sum of plane waves, that is $\psi(\mathcal{O}_c) = \sum_i a_i e^{i\mu_i \mathcal{O}_c/2}$ and matter states of the form $\psi(\mathcal{O}_\varphi) = \sum_{n=0}^{\infty} \alpha_n \psi_n$ with $\sum_{n=0}^{\infty} |\alpha_n|^2 < \infty$.

Let us briefly discuss how the elementary operators act on the physical Hilbert space $\mathcal{H}_{\text{phys}}$. The operators corresponding to the Dirac observables of the holonomy and fluxes denoted by $\hat{O}_{N_\mu}$ and $\hat{O}_p$ respectively act on the states $\Psi(\mathcal{O}_c, \mathcal{O}_\varphi)$ by multiplication and differentiation respectively on $\mathcal{H}_{\text{phys,grav}}$, and trivially on $\mathcal{H}_{\text{phys,} \varphi}$:

$$
\hat{O}_{N_\mu} \Psi(\mathcal{O}_c, \mathcal{O}_\varphi) := (\hat{O}_{N_\mu} \otimes 1) \Psi(\mathcal{O}_c, \mathcal{O}_\varphi) = e^{i\mu \mathcal{O}_c/2} \psi(\mathcal{O}_c) \otimes \psi(\mathcal{O}_\varphi),
\hat{O}_p \Psi(\mathcal{O}_c, \mathcal{O}_\varphi) := (\hat{O}_p \otimes 1) \Psi(\mathcal{O}_c, \mathcal{O}_\varphi) = -i \frac{8\pi \gamma \ell_p^2}{3} \frac{d}{d\mathcal{O}_c} \psi(\mathcal{O}_c) \otimes \psi(\mathcal{O}_\varphi).
$$

Likewise the elementary operators corresponding to the Dirac observables $\mathcal{O}_\varphi, \mathcal{O}_{\pi \varphi}$ which we denote by $\hat{\mathcal{O}}_{\varphi}$ and $\hat{\mathcal{O}}_{\pi \varphi}$ respectively act trivially on $\mathcal{H}_{\text{phys,grav}}$ and as multiplication and derivative operators respectively on $\mathcal{H}_{\text{phys,} \varphi}$, with an explicit action of the form:

$$
\hat{\mathcal{O}}_{\varphi} \Psi(\mathcal{O}_c, \mathcal{O}_\varphi) := (1 \otimes \hat{\mathcal{O}}_{\varphi}) \Psi(\mathcal{O}_c, \mathcal{O}_\varphi) = \psi(\mathcal{O}_c) \otimes \mathcal{O}_\varphi \psi(\mathcal{O}_\varphi),
\hat{\mathcal{O}}_{\pi \varphi} \Psi(\mathcal{O}_c, \mathcal{O}_\varphi) := (1 \otimes \hat{\mathcal{O}}_{\pi \varphi}) \Psi(\mathcal{O}_c, \mathcal{O}_\varphi) = \psi(\mathcal{O}_c) \otimes \frac{\hbar}{i} \frac{d}{d\mathcal{O}_\varphi} \psi(\mathcal{O}_\varphi).
$$

In the following, as often done in physics notation, we will suppress the tensor product and work with the notation on the left hand side of the equations above and the action of the corresponding operators is always understood in the sense defined above.

As in unreduced LQC, we would be working with the triad (or volume) representation in which the operator $\hat{O}_{N_\mu}$ acts as a translation operator

$$
\hat{O}_{N_\mu} \Psi(p, \mathcal{O}_\varphi) = \Psi(p + \mu^\prime, \mathcal{O}_\varphi) = \Psi(p + \mu^\prime, \mathcal{O}_\varphi)
$$
and \( \hat{O}_p \) acts as a multiplication operator

\[
\hat{O}_p \Psi(\mathcal{O}_p, \mathcal{O}_\varphi) = \frac{8 \pi \gamma \ell_p^2}{6} \mu \Psi(\mathcal{O}_p, \mathcal{O}_\varphi).
\] (3.9)

Note that since there are no fermions in our analysis, as in LQC, we consider states \( \Psi(\mathcal{O}_p, \mathcal{O}_\varphi) \) such that they are symmetric under parity operation: \( \hat{\Pi} \Psi(\mathcal{O}_p, \mathcal{O}_\varphi) = \Psi(-\mathcal{O}_p, \mathcal{O}_\varphi) \), i.e. they satisfy \( \Psi(\mathcal{O}_p, \mathcal{O}_\varphi) = \Psi(-\mathcal{O}_p, \mathcal{O}_\varphi) \).

The gravitational part of the Hamiltonian, denoted by \( H_{\text{phys}}^{\text{grav}} \), is obtained by expressing terms involving the symmetry reduced connection in terms of holonomies along the edges of a square with comoving length \( \ell \mathcal{O}_V_{1/3} \). In terms of the Dirac observables, the gravitational part in the classical theory can be written as

\[
H_{\text{phys}}^{\text{grav}} = \lim_{\ell \to 0} \sin(\ell \mathcal{O}_c) \left[ -\frac{\text{sgn}(\mathcal{O}_p)}{32 \pi^2 G^2 \gamma^3 \ell^3} \sum_k \text{Tr}_\mathcal{R} \hat{O}_k \{ \mathcal{O}_k^{-1}, \mathcal{O}_p^{3/2} / \mathcal{O}_p \} \right] \sin(\ell \mathcal{O}_c) .
\] (3.10)

Here in contrast to unreduced LQC \([11]\), \( H_{\text{phys}}^{\text{grav}} \) is expressed in terms of Dirac observables. In particular, \( H_{\text{phys}}^{\text{grav}} \) is the Dirac observable of the rescaled gravitational contributions to the Hamiltonian constraint denoted by \( C_{\text{grav}}^{16 \pi G} \) in \([11]\). We will denote the corresponding operator on the physical Hilbert space \( \mathcal{H}_{\text{phys}} \) by \( \hat{H}_{\text{phys,grav}}^{\text{grav}} \) which is a true Hamiltonian in our approach, whose action on physical states does not vanish in the physical Hilbert space. In contrast to this in \([11]\) Dirac quantization was applied for the \( k = 0 \) FLRW model sourced with a massless scalar field used as a relational clock and consequently the quantization of \( C_{\text{grav}}^{16 \pi G} \) was performed which vanishes in the quantum theory.

Let us recall that in LQC, \( \ell \) is chosen to coincide with the physical length of the square loop with area given by the minimum area eigenvalue in LQG. In the improved dynamics prescription of \([11]\), which is the only physically viable prescription in the isotropic case \([65]\), this physical length is measured by \( \bar{\mu} = \sqrt{\Delta / \mathcal{O}_p} \) with \( \Delta = 4 \sqrt{3} \pi^2 \ell_p^2 \). Since \( \bar{\mu} \) depends on the triad \( \mathcal{O}_p \), the holonomy operator \( \hat{O}_k^{(\mu)} \) when restricted to \( \mathcal{H}_{\text{phys,grav}} \) is the shift operator on eigenstates of the volume operator \( |\nu\rangle \) where \( \nu = K \text{sgn}(\mu) |\mu|^{3/2} \) with \( K = \frac{2 \sqrt{7}}{3 \sqrt{3}} \) and acts trivially on \( \mathcal{H}_{\text{phys,grav}} \). For this reason, it is convenient to switch from the triad to the volume representation in \( \mathcal{H}_{\text{phys,grav}} \) (see \([11]\) for more details). In this case

\[
\mathcal{H}_{\text{phys,grav}} = \text{span}(|\nu\rangle : \nu \in \mathbb{R}) \quad \text{with} \quad \langle \nu, \nu' \rangle = \delta_{\nu \nu'}.
\] (3.11)

When acting on the volume-kets in \( \mathcal{H}_{\text{phys,grav}} \), the action of the operator corresponding to the Dirac observables for the volume, defined as \( \hat{\mathcal{O}}_V = \bar{\mathcal{O}}_p^{3/2} \), and holonomy operators is given by

\[
\hat{\mathcal{O}}_V |\nu\rangle = \left( \frac{8 \pi G \gamma}{6} \right)^{3/2} \frac{|\nu|}{K} |\nu\rangle, \quad \hat{\mathcal{O}}_p |\nu\rangle = |\nu + 1\rangle.
\] (3.12)

Further, the holonomy operator acts trivially on \( \mathcal{H}_{\text{phys,grav}} \).

The corresponding quantum operator for the gravitational part of the physical Hamiltonian acting on \( \mathcal{H}_{\text{phys}} \), following the construction in \([11]\), becomes

\[
\hat{H}_{\text{phys}}^{\text{grav}} \Psi(\mathcal{O}_V, \mathcal{O}_\varphi) := \left( \hat{H}_{\text{phys}}^{\text{grav}} \otimes \mathbb{1} \right) \Psi(\mathcal{O}_V, \mathcal{O}_\varphi)
= \left( \sin \left( \bar{\mu} \mathcal{O}_c \right) \left[ \frac{3 \text{sgn}(\mathcal{O}_V)}{16 \pi^2 G^2 \gamma^3 \bar{\mu}^3} \left( \sin \left( \frac{\bar{\mu} \mathcal{O}_c}{2} \right) \hat{\mathcal{O}}_V \cos \left( \frac{\bar{\mu} \mathcal{O}_c}{2} \right) \right) \right] \sin \left( \bar{\mu} \mathcal{O}_c \right) \Psi(\mathcal{O}_V) \otimes \Psi(\mathcal{O}_\varphi) .
\] (3.13)
The quantization of the matter part of the Hamiltonian $\hat{H}^\varphi_{\text{phys}}$ with a scalar field $\varphi$ in an inflationary potential $U(\mathcal{O}_\varphi)$ yields

$$\hat{H}^\varphi_{\text{phys}} \Psi(\mathcal{O}_V, \mathcal{O}_\varphi) = \left( -\frac{\hbar^2}{2} \tilde{\mathcal{P}}^{3/4}_{[\mathcal{O}_{\mathcal{V}}]} \tilde{\mathcal{P}}^{3/4}_{[\mathcal{O}_{\mathcal{\varphi}}]} + \mathcal{O}_{[\mathcal{P}_{\mathcal{V}}]}^{3/4} U(\tilde{\mathcal{O}}_{\varphi}) \mathcal{O}_{[\mathcal{P}_{\mathcal{\varphi}}]}^{3/4} \right) \Psi(\mathcal{O}_V, \mathcal{O}_\varphi),$$

where we chose a symmetric operator ordering.

Given these two individual contributions, the physical Hamiltonian in both dust models is just given by

$$\hat{H}_{\text{phys}} = \hat{H}^{\text{grav}}_{\text{phys}} + \hat{H}^\varphi_{\text{phys}}.$$

At the classical level in the reduced phase space $\hat{H}_{\text{phys}}$ is generating the equations of motion of the elementary Dirac observables $(\mathcal{O}_b, \mathcal{O}_V, \mathcal{O}_\varphi, \mathcal{O}_\pi)$. At the quantum level this yields the Heisenberg equations for the corresponding operators of these Dirac observables. Switching from the Heisenberg picture to the Schrödinger picture we can then find for the dust reference models the respective quantum gravitational Schrödinger-like equations given by

$$i\hbar \frac{\partial}{\partial \tau} \Psi(\mathcal{O}_V, \mathcal{O}_\varphi; \tau) = \left( \hat{H}^{\text{grav}}_{\text{phys}} + \hat{H}^\varphi_{\text{phys}} \right) \Psi(\mathcal{O}_V, \mathcal{O}_\varphi; \tau).$$

Using the action of $\hat{H}^{\text{grav}}_{\text{phys}}$ and $\hat{H}^\varphi_{\text{phys}}$, one finds that,

$$\hat{H}_{\text{phys}} \Psi(\mathcal{O}_V, \mathcal{O}_\varphi; \tau) = \left( \hat{H}^{\text{grav}}_{\text{phys}} + \hat{H}^\varphi_{\text{phys}} \right) \Psi(\mathcal{O}_V, \mathcal{O}_\varphi; \tau)
= -\alpha B(\mathcal{O}_V) \partial^2_{\mathcal{O}_\varphi} \Psi(\mathcal{O}_V, \mathcal{O}_\varphi; \tau) - \frac{|\mathcal{O}_V|}{2\alpha K} U(\mathcal{O}_\varphi) \Psi(\mathcal{O}_V, \mathcal{O}_\varphi; \tau)
- \alpha C^+(\mathcal{O}_V) \Psi(\mathcal{O}_{V+4}, \mathcal{O}_\varphi; \tau) - \alpha C^0(\mathcal{O}_V) \Psi(\mathcal{O}_V, \mathcal{O}_\varphi; \tau)
- \alpha C^-(\mathcal{O}_V) \Psi(\mathcal{O}_{V-4}, \mathcal{O}_\varphi; \tau),$$

with coefficients given by

$$\alpha = \frac{1}{2} \left( \frac{6}{8\pi G\gamma} \right)^{3/2}, \quad B(\mathcal{O}_V) = \left( \frac{3}{2} \right)^3 K|\mathcal{O}_V|||\mathcal{O}_V + 1|^{1/3} - |\mathcal{O}_V - 1|^{1/3}|^3,$$

$$C^+(\mathcal{O}_V) = \frac{3\pi K G}{8} |\mathcal{O}_V + 2|||\mathcal{O}_V + 1| - |\mathcal{O}_V + 3||,$$

$$C^-(\mathcal{O}_V) = C^+(\mathcal{O}_V - 4), \quad C^0(\mathcal{O}_V) = -C^+(\mathcal{O}_V) - C^-(\mathcal{O}_V).$$

The expressions of $C^+$, $C^0$ and $C^-$ are same as in unreduced LQC [41] albeit with generalization to observables. Here as in Dirac quantization of LQC we have expressed the inverse volume in the kinetic energy term of scalar field using Thiemann identity [75], which results in

$$\tilde{\mathcal{O}}_{\mathcal{V}-1} \Psi(\mathcal{O}_V, \mathcal{O}_\varphi; \tau) = B(\mathcal{O}_V) \Psi(\mathcal{O}_V, \mathcal{O}_\varphi; \tau),$$

with $B(\mathcal{O}_V)$ given by the expression above in [3.18]. We thus obtain the evolution equation as a second order quantum difference equation with the same uniform spacing in volume as in conventional LQC which is non-singular. Note that the physical Hamiltonian only relates states which are supported on a ‘lattice’: $\mathcal{L}_\pm = \{\nu = \pm (4n + \epsilon)\}$ with $n \in \mathbb{N}$ and $\epsilon \in (0, 4]$. One can then choose a particular ‘lattice’, and as in unreduced LQC, one expects that the action of the physical Hamiltonian and the Dirac observable operators preserve the chosen ‘lattice’. The coefficients $C^+(\mathcal{O}_V)$, $C^0(\mathcal{O}_V)$ and $C^-(\mathcal{O}_V)$ do not vanish on any chosen ‘lattice’. Thus, given the wavefunction at volumes $\mathcal{O}_{V^*+4}$ and $\mathcal{O}_{V^*}$ for $V^*$ lying in the chosen lattice, the quantum difference equation
recursively determines the wavefunction at volume $O_{V=-4}$. The quantum difference equation allows to determine the wavefunction across the to-be classical singularity at zero volume, and in this sense, there is a resolution of big bang singularity at this level.

As shown in [76], the physical Hamiltonian operator of the dust models $\hat{H}_{\text{phys}}$ is self-adjoint in $H_{\text{phys}} = H_{\text{phys,grav}} \otimes H_{\text{phys,ϕ}}$ which is the physical Hilbert space in the dust models. Note that in [76] only the case of a massless scalar field with a cosmological constant was considered, however as discussed in [30] the property of self-adjointness is preserved for any non-exotic matter contribution added to the gravitational sector. One can include potentials in this setting which are equivalent to adding different cosmological constants for different time slices. Using above results, self-adjointness of the physical Hamiltonian follows. Further, also the elementary Dirac observables $\hat{O}_V, \hat{O}_b, \hat{O}_ϕ, \hat{O}_π$ are self-adjoint operators in $H_{\text{phys}}$ and the physical Hamiltonian $\hat{H}_{\text{phys}}$ can then be understood as a function of these elementary operators.

Thus using the dust reference fields as clocks we have found the corresponding quantum gravitational Schrödinger-like equation which is a difference equation with a uniform spacing in four Planck volumes. The latter is a primary characteristic of the LQC quantum difference equation in the $\mu$-scheme which results in a successful resolution of the big bang singularity replacing it with a quantum bounce [41, 42]. In contrast to the unreduced LQC model [41], in the dust models we can without further technical complications include a potential for the inflaton since even then the resulting physical Hamiltonian operator stays time-independent. As mentioned before in the model of type II [30, 31] this would be also possible but up to now an analysis of the physical properties of such a model is not available in the literature.

An important next step will be to investigate solutions of the above Schrödinger equation. Compared to the unreduced LQC model this is technically more involved since we have one more degree of freedom at the level of the physical Hilbert space. As a result, numerical simulations with the full quantum difference equation will be more demanding. Nevertheless, thanks to recent developments in including supercomputing efforts in LQC [77] and efficient algorithms [78], the situation above is expected to be no more than computational requirements of analyzing difference equations in anisotropic models which have been successfully analyzed recently [79]. We expect that as in conventional LQC, numerical simulations with quantum difference equations would show that singularity resolution occurs via a quantum bounce in the Planck regime. Note that since we use the usual kinematical LQC representation for $H_{\text{phys}}$ here the physical Hilbert space on which the Schrödinger-like equation is formulated is still non-separable. However, given the structure of the quantum difference equation discussed above regarding ‘lattices’ $L_{±\epsilon}$, we expect that if we restrict on solutions of the quantum dynamics there is a super-selection and a Hilbert space associated to the solutions can become separable.

### III.B. The physical Hilbert space and Hamiltonian in the Klein-Gordon scalar field model

After discussing the quantum dynamics of the two dust models in detail in the last subsection we will be brief in the presentation of the Klein-Gordon scalar field model where many of the steps performed in the dust models can be carried over. We consider the same $H_{\text{phys,ϕ}}$ for the inflaton but slightly modify the inner product for the gravitational part and introduce as in [41] the following inner product:

$$H_{\text{phys,grav}}^B := \text{span}(|ν⟩ : ν ∈ \mathbb{R}) \quad \text{with} \quad ⟨ν, ν'⟩_B := ⟨ν, B(O_V)ν'⟩,$$

where $B(O_V)$ is given in (3.18). The reason for this modification is that we want the physical Hamiltonian of the scalar field model to be self-adjoint. The elementary operators acting on $H_{\text{phys}}$ act in a similar way as in the dust model shown in (3.6) and (3.7) respectively. As before we can
go from the Heisenberg picture that one obtains after the reduced phase space quantization to the Schrödinger picture. In case of the Klein-Gordon scalar field clock, the Schrödinger-like equation is given by

\[
i\hbar \frac{\partial}{\partial \tau} \Psi(O_V, O_\phi; \tau) = \sqrt{\left| -2\hat{B}^{-1}(O_V)(\hat{H}^{grav}_{phys} + \hat{H}^\phi_{phys}) \right|} \Psi(O_V, O_\phi; \tau)
\]

(3.21)

with the action of \((\hat{H}^{grav}_{phys} + \hat{H}^\phi_{phys}))\Psi(O_V, O_\phi; \tau)\) given by (3.17). Here the factor of \(B(O_V)^{-1}\) arises from the inverse volume term in the Klein-Gordon clock and we included in absolute value for the expression under the square root.

The operator under the square root inside the absolute value, up to the factor 2, can be identified with the \(\hat{\Theta}\) operator in [41] written in terms of Dirac observables and generalized to the case of an inflationary potential. As discussed in the case of the dust model, and shown in [76] this is a self-adjoint operator on the physical Hilbert space \(H_{phys}\). In this case, unlike the dust models, the spectrum of the physical Hamiltonian is expected to be more non-trivial capturing some features discussed earlier for a positive cosmological constant with a massless scalar field as a clock [46, 47] but now with an additional complexity of a potential which corresponds to choosing different values of a positive cosmological constant at different times \(\tau\). Further, unlike the dust clock, we now have a square root operator arising from the physical Hamiltonian in this case. Hence, the structure of the Schrödinger equation of the scalar field model appears more complicated compared to the dust model case at this stage. We found above that the evolution equation in the reduced phase quantization turns out to be a quantum difference equation with a quantum discreteness set by the underlying quantum geometry via the minimum eigenvalue of the area operator in LQG. This is the same structure as in conventional LQC which results in a singularity resolution.

### III.C. Effective dynamical equations for the dust clocks

As in the Dirac quantization of LQC, insights into the physical evolution can be obtained by using an effective spacetime description which captures the quantum evolution in LQC for different models quite accurately [40, 77, 79, 80]. This effective description allows obtaining numerical solutions on a differentiable spacetime which encodes quantum gravitational effects. In standard LQC this effective spacetime description is obtained from a geometrical formulation of the quantum theory using sharply peaked states which finally results in an effective Hamiltonian constraint. For the spatially flat models, it turns out that this effective Hamiltonian constraint can be viewed as obtained by replacing symmetry reduced connection variable \(c\) in the classical Hamiltonian constraint with \(\sin(\bar{\mu}c)\) [81]. In the following we assume an effective spacetime description to exist in the reduced phase space quantization presented above for dust and Klein-Gordon reference fields. In this setting we first present dynamical equations for dust clocks, which is followed by those for Klein-Gordon scalar field clock. As in the usual case in LQC, we work in the approximation where effects from inverse volume operators which are significant only near the Planck volume can be ignored. In the solutions discussed below, the volume of the universe remains much larger than the Planck volume even at bounce which is consistent with above approximation. Further, we will choose the orientation of the triad to be positive.

For the dust clock, following the procedure used in Dirac quantization in LQC, an effective physical Hamiltonian written in terms of Dirac observables \(O_V, O_b, O_\phi,\) and \(O_{\pi_\phi}\), can be written as:

\[
H_{eff}^{FLRW, dust} = -\frac{3O_V}{8\pi G\lambda^2\gamma^2} \sin^2(\lambda O_b) + \frac{O_{\pi_\phi}^2}{2O_V} + O_V U(O_\phi),
\]

(3.22)
where \( \mathcal{O}_b \) is defined as
\[
\mathcal{O}_b = \mathcal{O}_c / |\mathcal{O}_c|^{1/2}
\]
and \( \mathcal{O}_V = \text{sgn}(\mathcal{O}_p)\mathcal{O}_c^{3/2} \) and \( \lambda = \sqrt{\Delta} \). One can then use \( \mathcal{O}_b \) and \( \mathcal{O}_V \) as phase space variables, which satisfy \( \{\mathcal{O}_b, \mathcal{O}_V\} = 4\pi G\gamma \). The resulting Hamilton’s equations in the reduced phase space are
\[
\frac{d\mathcal{O}_V}{d\tau} = \frac{3\mathcal{O}_V}{2\lambda\gamma} \sin(2\lambda\mathcal{O}_b),
\]
\[
\frac{d\mathcal{O}_b}{d\tau} = -\frac{3\sin^2(\lambda\mathcal{O}_b)}{2\gamma\lambda^2} - 4\pi G\gamma \mathcal{O}_p^\varphi,
\]
\[
\frac{d\mathcal{O}_\pi^\varphi}{d\tau} = \frac{\mathcal{O}_\pi^\varphi}{\mathcal{O}_V},
\]
\[
\frac{d\mathcal{O}_\pi^\varphi}{d\tau} = -\mathcal{O}_V \frac{dU(\mathcal{O}_\varphi)}{d\mathcal{O}_\varphi}.
\]
Here \( \mathcal{O}_p^\varphi \) denotes the observable corresponding to the pressure of the inflaton field \( \varphi \)
\[
\mathcal{O}_p^\varphi = \frac{\mathcal{O}_\pi^\varphi}{2\mathcal{O}_V^2} - U(\mathcal{O}_\varphi).
\]
Since the dust clocks are pressure-less they do not contribute to total pressure which is captured by the above observable. In contrast, the total energy density observable also includes contribution from the dust:
\[
\mathcal{O}_\rho = \frac{\mathcal{O}_\pi^\varphi}{2\mathcal{O}_V^2} + U(\mathcal{O}_\varphi) + \frac{\mathcal{E}_\text{dust}}{\mathcal{O}_V},
\]
where \( \mathcal{E}_\text{dust} \) is defined as the negative physical Hamiltonian given by \( (3.22) \), and the ratio \( \mathcal{E}_\text{dust} / \mathcal{O}_V \) corresponds to the energy density of the dust clock. Note that in the Brown-Kuchař case, the energy density for dust can also take negative values.

For understanding cosmological dynamics it is useful to derive the modified Friedmann equation which can be obtained from \( (3.23) \) by computing the square of the observable for the Hubble rate \( H = \dot{V}/3V \), which using \( (3.22) \) yields
\[
\mathcal{O}_H^2 = \frac{\dot{\mathcal{O}}_V^2}{9\mathcal{O}_V^2} = \frac{8\pi G}{3} \mathcal{O}_\rho \left(1 - \frac{\mathcal{O}_\rho}{\rho_{\text{max}}}\right).
\]
Here \( \rho_{\text{max}} \) is a constant determined by the area gap,
\[
\rho_{\text{max}} = \frac{3}{8\pi G\gamma^2\lambda^2}.
\]
When \( \mathcal{O}_\rho = \rho_{\text{max}} \approx 0.41\rho_{\text{Pl}} \), the observable corresponding to the Hubble rate vanishes and the Dirac observable of the volume \( \mathcal{O}_V \) reaches its minimum value when the bounce occurs. At this value the energy density is bounded above by \( \rho_{\text{max}} \). In the limit where \( \lambda \to 0 \), \( \rho_{\text{max}} \to \infty \) and the observable \( \mathcal{O}_\rho \) is unbounded from above. In this limit, the big bang singularity is recovered.

As compared with the modified Friedmann equation obtained in an effective description of the Dirac quantization of LQC, equation \( (3.29) \) has the same form and the same maximum energy density at which the bounce takes place. The only difference lies in the composition of the energy density which is now made up of two ingredients, the inflaton and the contribution from dust clock. It is also straightforward to show that the form of the modified Raychaudhuri equation in the relational formalism is the same as its counterpart in LQC. This is owing to the property of the observable map in \( (3.2) \) which ensures all the dynamical equations can be lifted to the observable
level in a straightforward way once the contribution from the dust field to the total energy density is taken into account.

Finally, the Klein-Gordon equation of the scalar fields can be derived from the Hamilton’s equations in a straightforward way. Taking the time derivative of (3.25) and combining it with (3.26), one finds,

\[ \ddot{\mathcal{O}} + 3\mathcal{O}_H \dot{\mathcal{O}} + U,\mathcal{O} = 0. \]  

(3.31)

Using this equation it is straightforward to show that the continuity equation is satisfied for the observables of energy density and pressure of the scalar field. Further, the observable for the total energy density which includes contribution from dust clocks also satisfies the continuity equation.

In the next section, we use these dynamical equations to understand some features of the resulting non-singular dynamics with dust clocks.

### III.D. Effective dynamical equations for the Klein-Gordon scalar field clock

Similar to the dust model, we assume that an effective spacetime description also exists in the Klein-Gordon scalar field clock model. By using the \( \mathcal{O}_b, \mathcal{O}_V \) variables and the same substitutions in the classical physical Hamiltonian \( \mathcal{H}_{\text{eff}} \), the effective Hamiltonian in the Klein-Gordon scalar field model can be shown to be

\[ \mathcal{H}_{\text{eff}, \text{FLRW, scalar}} = \sqrt{-2\mathcal{O}_V \left( -\frac{3\mathcal{O}_V}{8\pi G\lambda^2 \gamma^2} \sin^2(\lambda \mathcal{O}_b) + \frac{\mathcal{O}_\pi^2}{2\mathcal{O}_V} + \mathcal{O}_V U(\mathcal{O}_\phi) \right)}, \]  

(3.32)

It is then straightforward to derive Hamilton’s equations which read

\[ \frac{d\mathcal{O}_V}{d\tau_\chi} = \frac{3\mathcal{O}_N \mathcal{O}_V}{2\lambda \gamma} \sin(2\lambda \mathcal{O}_b), \]  

(3.33)

\[ \frac{d\mathcal{O}_b}{d\tau_\chi} = -4\pi G \gamma \mathcal{O}_N \left( \mathcal{O}_\rho^{\text{scalar}} + \mathcal{O}_p^{\text{scalar}} \right), \]  

(3.34)

\[ \frac{d\mathcal{O}_\phi}{d\tau_\chi} = \frac{\mathcal{O}_N \mathcal{O}_\pi^2}{\mathcal{O}_V}, \]  

(3.35)

\[ \frac{d\mathcal{O}_\pi}{d\tau_\chi} = -\mathcal{O}_N \mathcal{O}_V \frac{dU(\mathcal{O}_\phi)}{d\mathcal{O}_\phi}, \]  

(3.36)

where \( \mathcal{O}_N = -\mathcal{O}_V / \mathcal{H}_{\text{eff}, \text{FLRW, scalar}} \) and the total energy density and the pressure are given by

\[ \mathcal{O}_\rho^{\text{scalar}} = \frac{\mathcal{O}_\pi^2}{2\mathcal{O}_V^2} + U(\mathcal{O}_\phi) + \frac{\mathcal{E}_\chi^2}{2\mathcal{O}_V^2}, \]  

(3.37)

\[ \mathcal{O}_p^{\text{scalar}} = \frac{\mathcal{O}_\pi^2}{2\mathcal{O}_V^2} - U(\mathcal{O}_\phi) + \frac{\mathcal{E}_\chi^2}{2\mathcal{O}_V^2}. \]  

(3.38)

In the above formulas, \( \mathcal{E}_\chi = -\mathcal{H}_{\text{eff}, \text{FLRW, scalar}} \) is a constant of motion. It should be noted that in the Hamilton’s equations all the Dirac observables are evolved with respect to the Klein-Gordon scalar physical time \( \tau_\chi \). This physical time is related to the physical dust time \( \tau \), which is proper time, by

\[ \frac{d\tau}{d\tau_\chi} = \mathcal{O}_N. \]  

(3.39)
Further, given that the lapse function is negative, \( \tau_\chi \) is negative of the scalar field clock used in LQC \[11\].

The Friedmann and Raychaudhuri equations with respect to the Klein-Gordon scalar physical time \( \tau_\chi \) are slightly different than those with respect to the dust physical time \( \tau \). For example, with respect to the Klein-Gordon scalar field clock, the Friedmann equation in effective description takes the form

\[
\tilde{H}^2 = O_N^2 \frac{8\pi G}{3} O_\rho \left(1 - \frac{O_\rho}{\rho_{\text{max}}} \right).
\] (3.40)

Here in order to distinguish it from the Hubble rate in the dust models, we defined the Hubble rate in the Klein-Gordon scalar field model as \( \tilde{H} = dO_V/d\tau_\chi \). Note that the above equation still yields the bounce at the maximum energy density given by (3.30) and the super-inflationary phase, defined as the regime in which the time derivative of the Hubble rate is positive, occurs in the range \( \rho_{\text{max}}/2 \leq O_\rho^{\text{scalar}} \leq \rho_{\text{max}} \).

One can also study the evolution in \( \tau \) which is a monotonic function of \( \tau_\chi \). Then the dynamical equations of the fundamental observables take the same form as those in the dust models, but, the difference lies in the expression of the energy density and pressure which carry the fingerprints of the different types of clocks. Also with respect to the dust physical time \( \tau \), the modified Friedmann and Raychaudhuri equations take the same forms as those in LQC. Further, the Klein-Gordon equation of the massive scalar field \( O_\phi \) will take the same form as (3.31) in the physical dust time \( \tau \). For this reason, in the following section, we understand physical implications for this model using time \( \tau_\chi \) but also discuss some results in time \( \tau \).

Finally to summarize, in this section, using the techniques from LQC, we have quantized the reduced phase space of a spatially flat FLRW universe with both dust clocks and a massless Klein-Gordon scalar clock. We have derived the Schrödinger-like quantum difference equations and the Hamilton’s equations of the effective dynamics for the three different types of clocks. These effective equations lay the basis for the numerical analysis of the background dynamics of the spatially flat FLRW universe in the reduced phase space framework which is discussed in the following.

### IV. NUMERICAL ANALYSIS OF THE EFFECTIVE DYNAMICS WITH THE DUST AND MASSLESS KLEIN-GORDON SCALAR FIELD CLOCKS

In this section, starting from the Hamilton’s equations obtained in an effective spacetime description of the reduced phase quantization of a flat FLRW universe, numerical solutions of the background dynamics are found when a single scalar field is minimally coupled to gravity. We discuss two separate cases: one for dust clocks as reference fields and another one with a Klein-Gordon scalar reference field. The inflationary potential is chosen to be the Starobinsky potential

\[
U = \frac{3m^2}{16\pi G} \left(1 - e^{-\sqrt{\frac{16\pi G}{3}} O_\phi} \right)^2,
\] (4.1)

which is favored by the Planck data for the cosmic microwave background.\(^4\) From the observational constraints on the amplitude of the primordial scalar power spectrum \( A_s \) and the scalar spectral index \( n_s \) given by the values

\[
A_s = 2.10 \times 10^{-9}, \quad n_s = 0.96,
\] (4.2)

\(^4\) Note that unlike the conventional derivation, the Starobinsky potential is not derived in LQC from a higher curvature term in the action. Rather, as in other works in LQC we consider it as a phenomenological input. For a discussion of higher curvature terms in the action framework of LQC, see \[82\].
we can fix the mass of the scalar field to be $m = 2.44 \times 10^{-6}$. We choose the initial conditions at the bounce where the total energy density reaches its maximum value. A property of the physical Hamiltonian in this reduced phase quantization is that at the bounce $O_b = \pi/2\lambda$. This leaves the Dirac observables $O_V$, $O_\varphi$ and $O_{\pi\varphi}$ to be specified for the initial conditions. For our numerical solutions, we set the Dirac observable of the volume at the bounce to $10^3$ in Planck units. Then the choice of the initial values of $O_\varphi$ and $O_{\pi\varphi}$ determines the value of the physical Hamiltonian at the bounce, or equivalently, the initial value of $E_{\text{dust}}$ in the dust model and $E_\chi$ in the Klein-Gordon scalar field model. Apart from studying singularity resolution with different clocks, we will be also interested in understanding the way energy density of the different clocks may have any imprint on the cosmological dynamics. For this reason, we parametrize the space of the initial conditions by $(O_\varphi, O_{\rho\text{clock}})$. We emphasize that the Dirac observable for the energy density of the clocks $O_{\rho\text{clock}}$ is a function of the Dirac observables $O_V$, $O_b$, $O_\varphi$ and $O_{\pi\varphi}$, given by $E_{\text{dust}}/O_V$ and $E_\chi^2/2O_V^2$ for the dust and the Klein-Gordon scalar field clocks respectively.

The effects of the dust reference fields on the background dynamics in the classical theory for both Gaussian and Brown-Kuchař dust models were discussed recently by the authors in [65]. There it was found that changing the initial dust energy density can effectively change the inflationary e-foldings. The numerical analysis of the classical theory in [65] started with initial conditions when the inflaton starts from the left wing of the Starobinsky potential as in this manuscript. It was found that increasing the positive dust energy density can decrease the inflationary e-foldings while increasing the magnitude of the negative dust energy density can have an opposite effect as long as the qualitative dynamics of the background evolution is not altered by the presence of the dust reference fields. When the magnitude of the initial negative dust energy exceeds an upper bound determined by the initial conditions for the other physical quantities, the inflationary phase is replaced by a recollapse of the universe which finally results in a big crunch singularity. In classical cosmology, solutions with either positive or negative dust energy density are past incomplete with an inevitable big bang singularity when evolved backward in time. In the following, we will show that all singularities encountered in the classical theory in [65] are resolved and replaced by a quantum bounce when the classical spatially flat FLRW spacetime is loop quantized as in the last section. Since after the bounce the dynamics of the universe is quickly approximated by the classical theory, the number of e-foldings in the slow-roll inflationary phase are quite similar in the classical theory and LQC when starting from the same initial conditions.

In the following we discuss some representative cases when the inflaton initially rolls down the left wing of the Starobinsky potential. Since the energy density of the dust field can also take negative values in the Brown-Kuchař dust model, we will consider both positive and negative dust energy densities in our analysis. Note that for the background dynamics of this cosmological model, both Gaussian and Brown-Kuchař dust clocks yield no difference when the energy density is positive. For this reason, in the following, cases for positive dust energy density we refer to both of the dust clocks. Further, in the discussion below all values of the Dirac observables are considered in Planck units.

### IV.A. Dust clocks with a positive energy density

In this subsection we discuss a representative case of initial conditions chosen for dust clocks with a positive energy density. As mentioned earlier, for numerical analysis we choose initial conditions for geometric variables as $O_{b_i} = \pi/2\lambda$ and $O_{V_i} = 1000$ in Planck units. Initial conditions for other variables are,

\[
O_{\varphi_i} = -1.45, \quad O_{\rho_i} = 10^{-8},
\]  

(4.3)
FIG. 1: In this figure, with the initial conditions given in (4.3), the evolution of the volume Dirac observable near the bounce is depicted in the top left panel where the inset figure shows the behavior of the Hubble rate across the bounce. The top right panel shows the Dirac observable of the volume at large times. The bottom left panels show the time evolution of the first slow-roll parameter till the end of inflation and the plot of kinetic and potential energies of the scalar field also expressed in terms of Dirac observables. The vertical lines in these graphs indicate the onset of inflation at $\tau = 3.17 \times 10^5$. The inflation ends at $\tau = 5.46 \times 10^7$, yielding a total of 63.1 inflationary e-foldings.

where the subscript ‘$i$’ stands for the initial values of the relevant quantities at the bounce. With these initial values, we find $O_{\pi\varphi_i} = 900$. Note that for the above initial conditions, $O_{\pi\varphi_i}$ can be either positive or negative, but the latter does not yield a viable phase of inflation and hence is not considered. Also, we choose these particular values for $O_{\varphi_i}$ and $O_{\pi\varphi_i}$ since they yield slightly greater inflationary e-foldings than 60 in LQC in the absence of dust reference fields. In particular, these initial conditions without any contribution from dust clocks yield 63.9 inflationary e-foldings (for details on number of e-foldings for various initial conditions in LQC for Starobinsky potential see [83]). One of our goals in the following will be to understand the effect of dust clocks on the number of e-foldings even when the energy density of clocks is much smaller than the inflaton energy density.

Fig. 1 shows the results for above initial conditions. In the top left panel of Fig. 1 we see that a non-singular bounce takes place at $\tau = 0$ with the inset showing the behavior of the Dirac observable for the Hubble rate. The super-inflationary phase starts from the bounce and ends at the moment when the Hubble rate reaches its maximum at around $\tau = 0.18$, yielding a total of 0.12 e-foldings. The universe at the bounce is dominated by the kinetic energy of the scalar field as shown in the plot of the kinetic and potential energy in the figure. As the inflaton first rolls down the left wing and then climbs up the right wing of the potential, it slows down with a positive velocity before the turnaround point. The slow-roll inflation takes place shortly after
the turnaround point and ends when the inflaton reaches the bottom of the potential. During the period from the bounce to the end of the inflation, the dust field plays a subdominant role as its energy density stays much less than the energy density of the scalar field. This behavior of the dust clocks becomes more obvious in the slow-roll inflationary phase. In this phase, the volume of the universe expands exponentially in the time measured by the dust clock, while the dust energy density decreases at the same rate as the inverse of the volume, in contrast to the almost constant potential energy of the scalar field during the slow-roll. The presence of the inflationary phase can be further confirmed by the plot of the observable for the slow-roll parameter $\mathcal{O}_{\epsilon H}$ defined as

$$\mathcal{O}_{\epsilon H} = \frac{4\pi G}{\mathcal{O}_H^2} \left( \mathcal{O}_{\rho,\phi} + \mathcal{O}_{\pi,\phi} + \mathcal{E}_{\text{dust}}^\mathcal{V} \right).$$  \hspace{1cm} (4.4)$$

Inflation starts at the moment when $\mathcal{O}_{\epsilon H} = 1$ as marked by the gray vertical line in the bottom left panel of Fig. 1 and ends when $\mathcal{O}_{\epsilon H}$ again equals unity after the onset of inflation. With the slow-roll approximation, one finds that the inflation ends when the value of the scalar field decreases to $\mathcal{O}_{\phi,\text{end}} = 0.19$ for the Starobinsky potential. The total number of inflationary e-foldings turns out to be 63.1 for the above chosen initial conditions.

![Graph](image)

**FIG. 2:** With the same initial conditions for the scalar field as in Fig. 1, the effect of the dust clocks on the number of e-foldings in the pre-inflationary phase ($N_{\text{pre}}$) and the slow-roll phase ($N_{\text{inf}}$) is depicted when the initial dust energy density is increased from $5 \times 10^{-8}$ to $10^{-4}$.

In order to study the effects of the dust fields on the background evolution of the universe, especially on the e-foldings in the pre-inflationary and the inflationary phase, we fix the value of the scalar field at the bounce as in (4.3) and change the initial dust energy density in small increments. Results are presented in Fig. 2, which shows that the e-foldings in the pre-inflationary phase increase with an increasing initial dust energy density at the bounce. Note that the pre-inflationary e-foldings are counted from the bounce to the onset of inflation, and includes the e-foldings from super-inflation. The e-foldings of the inflationary phase and the value of the scalar field at the onset of inflation are smaller for a larger initial dust energy density. This is because the Hubble friction becomes larger when the initial positive dust energy density is increased resulting in a smaller value of $\mathcal{O}_{\phi,\text{on}}$, the value of the field at which inflation starts. In the extreme case, when the initial dust energy is large enough so that the $\mathcal{O}_{\phi,\text{on}} \leq \mathcal{O}_{\phi,\text{end}}$, where $\mathcal{O}_{\phi,\text{end}}$ denotes the value of the field at the end of inflation, the inflationary phase disappears. Such extreme values clearly do not correspond to dust acting as a reference field and thus as a good clock. We find that these results are robust to changes in the value of $\mathcal{O}_{\phi,\text{i}}$. For a given value of $\mathcal{O}_{\phi,\text{i}}$ we find that there exists an upper bound on the value of energy density for which the inflationary phase does not occur in
LQC. For initial conditions considered in \((4.3)\), this bound turns out to be \(1.38 \times 10^{-4}\). Note that ideal dust reference clocks should behave as test fields with tiny energy densities compared to \(O_\phi\). For all such cases, our simulations show that dust energy density does not affect the e-foldings in various phases in a significant way.

**IV.B. Dust clocks with a negative energy density**

In the Brown-Kuchař model, the energy density of the dust can be negative. If the energy density of such a phantom dust is sufficiently large, the universe undergoes a recollapse before inflation can start. Classically such a universe encounters a big crunch singularity \(65\), which is avoided by loop quantum effects, and such initial conditions result in several cycles before inflation can start. Note that for the latter case, the Brown-Kuchař dust can not be considered as a good clock as it changes the qualitative dynamics significantly. Nevertheless, we discuss this case to show how different choices of initial conditions for the dust clock can result in very different dynamics. In the following, we first discuss a case when the energy density of dust allows inflationary dynamics to occur without any such cycles. This is followed by examples where the energy density of the dust clock is so negative that the universe undergoes a recollapse and cycles of contraction and expansion before inflation can set in.

\[
\begin{align*}
5 \times 10^4 & \quad 1 \times 10^5 \\
1 \times 10^5 & \quad 5 \times 10^5 \\
5 \times 10^5 & \quad 1 \times 10^6 \\
1 \times 10^6 & \quad 5 \times 10^6 \\
5 \times 10^6 & \quad 1 \times 10^7 \\
1 \times 10^7 & \quad 5 \times 10^7
\end{align*}
\]

**FIG. 3:** These plots correspond to the initial conditions given in \((4.5)\) for a negative energy density of the dust clock, the evolution of the volume Dirac observable and the Hubble rate is depicted near the bounce in the top left panel. The top right panel shows the evolution of the Dirac observable for the volume at large times until the end of inflation. The bottom panels show the time evolution of the first slow-roll parameter and the kinetic and potential energies of the scalar field. The vertical lines in these graphs indicate the onset of inflation at \(\tau = 3.18 \times 10^5\). Inflation ends at \(\tau = 5.60 \times 10^7\), yielding a total of 64.7 inflationary e-foldings.
The first set of initial conditions for negative energy density are chosen to differ from conditions in (4.3) just by a negative sign of the dust energy density,

\[ O_{\phi_i} = -1.45, \quad O_{\rho_{\text{dust}}^i} = -10^{-8}, \]

which also set \( O_{\kappa_{\phi_i}} = 900. \) Note that as before we choose \( O_{b_i} = \pi/2\lambda \) and \( O_{V_i} = 1000 \) in Planck units. In this case, the qualitative evolution of the universe is similar to the case with the positive dust energy density discussed in the last subsection. As shown in the top left panel of Fig. 3, the Dirac observables of the volume and the Hubble rate evolve continuously across the bounce which takes place at \( \tau = 0. \) Also, the dust field is subdominant at all times. The difference from Fig. 1 lies in the exact number of e-foldings of the inflationary phase, which in this case is 64.7, larger than the inflationary e-foldings in Fig. 1. This increase in the number of e-foldings is tied to the higher value of \( O_{\phi} \) at the onset of inflation when dust energy density is negative, which occurs because of the decrease in the Hubble friction when the inflaton climbs up the right wing of the potential. An increase in the magnitude of the negative dust energy density further decreases the Hubble friction which makes the inflaton turn around at a higher value of \( O_{\phi} \) in the Starobinsky potential. The effect of the dust energy density on the inflationary e-foldings is depicted in Fig. 4. We find that the number of e-foldings in the preinflationary phase decrease slightly when the magnitude of the initial dust energy density is increased. Increasing the magnitude of the negative dust energy density causes an increase in the value of the scalar field at the onset of inflation, and thus the total number of e-foldings of the inflationary phase increases. This behavior is opposite to what we found for the positive dust energy density. But similar to the latter case, for any given initial conditions, there is an upper bound \( O_{\rho_{\text{upper}}} \) (defined positive) on the magnitude of the negative dust energy density to ensure the dynamics of the LQC universe is not qualitatively altered by the presence of the dust reference field. When \( |O_{\rho_{\text{dust}}}^i| < O_{\rho_{\text{upper}}} \), the magnitude of the dust energy density is always smaller than that of the scalar field. If above condition is not met, the total energy density vanishes before the turnaround point occurs, leading to a recollapse of the universe.

![Graph](image-url)

**FIG. 4:** For the initial conditions as in Fig. 3, the effects of the dust field on the e-foldings is shown for the pre-inflationary and the inflationary phases. Our simulations show that unless the dust energy density becomes more negative than \(-5.35 \times 10^{-7}\) for the same initial conditions, the qualitative dynamics of the pre-inflationary phase is unaffected. Hence, we consider the interval as \( O_{\rho_{\text{dust}}}^i \in (-3 \times 10^{-7}, 10^{-9}) \).

From our simulations, we find that with the initial scalar field set to \( O_{\phi_i} = -1.45 \), the upper bound on the initial dust energy density turns out to be approximately \( O_{\rho_{\text{upper}}} = 5.35 \times 10^{-7} \). When \( |O_{\rho_{\text{dust}}}^i| > O_{\rho_{\text{upper}}} \), the universe undergoes a recollapse and a cyclic dynamics in LQC will appear.
This interesting case is not satisfied by ideal dust clocks because a relatively large magnitude of energy densities changes the universe with only one bounce into the one with many bounces. One such case occurs with the following initial conditions, chosen again with $O_{b_i} = \pi/2\lambda$ and $O_{V_i} = 1000$,

$$O_{\varphi_i} = -1.45, \quad O_{\rho_{dust}} = -5.35 \times 10^{-7},$$

which also set $O_{\pi_{\varphi}} = 900$. Results are presented in Fig. 5 in which the evolution of the Dirac observable of the volume and the scalar field is depicted. It can be seen from the figure that the universe experiences cycles of alternating expanding and contracting phases. During these cycles, a bounce occurs when the total energy density reaches the critical energy density $\rho_{\text{max}}$ in LQC whereas at the recollapse the positive energy density of the scalar field is canceled by the negative dust energy density. Meanwhile, the volume at successive recollapse points increases very slightly, making the kinetic energy of the scalar field also slightly decrease. This indicates a hysteresis-like phenomenon, which has been discussed recently in a closed universe in LQC [84]. In addition, the scalar field undergoes a step-like increase when the universe enters into alternating phases of expansion and contraction. At each bounce, the kinetic energy of the field increases causing a jump in the value of the scalar field. On the other hand, when the recollapse is approached, the kinetic energy is considerably smaller which makes the value of the scalar field change slowly in that regime. From our numerical solutions, we find that the cyclic universe without the inflationary phase continues until $t = 10^9$ (in Planck seconds). It is possible that after many bounces and recollapses, the inflation can still take place at a time when the dust energy density becomes less than the energy density of the scalar field in the expanding phase. However, due to the flatness of the Starobinsky potential on its right wing, the volume of the universe only changes slightly in each cycle, it possibly takes a very long period before the inflation finally sets in. This cyclic behavior of the universe caused by the negative dust energy density in the loop quantized model is in striking contrast with the behavior of the universe in the classical theory. As discussed in [65], in the classical FLRW universe, when the magnitude of the negative dust energy density is large enough to cancel the energy density of the scalar field, the universe recollapses and heads towards the big crunch singularity. However, we find in our case that this singularity is avoided because of quantum gravitational effects and the big crunch singularity is avoided, resulting in a cyclic evolution.

While above initial conditions do not easily lead to inflation in short time, it is not difficult to find initial conditions where inflation occurs after some cycles. An example is for the initial conditions:

$$O_{\varphi_i} = -2.52296, \quad O_{\rho_{dust}} = -10^{-6},$$

from which one can find $O_{\pi_{\varphi}} = 905$ using $O_{b_i} = \pi/2\lambda$ and $O_{V_i} = 1000$. The results are shown in Fig. 6. The left panel of Fig. 6 clearly shows that the largest value for the Dirac observable of the volume at different collapse points are changing slightly in the forward evolution. Meanwhile, the scalar field initially moves steadily in one direction when the universe is undergoing cycles of alternating expanding and contracting phases. However, when the inflation takes place, the inflaton reaches its turnaround point and the value of the scalar field starts to decrease. Afterwards, as the volume of the universe experiences an exponential expansion, the effects of the dust field becomes negligible as compared with the scalar field. From our simulations, we find that in order for the universe to transit from the cyclic phase to the inflationary phase, the slope of the scalar potential plays an important role. Unlike the Hubble friction which also assumes oscillating behavior in the cyclic phase, the potential related term in the Klein-Gordon equation (3.31) always acts as a frictional force when the scalar field steadily moves in the direction with increasing $O_{\varphi}$. The
FIG. 5: In this figure, the initial conditions are chosen as in (4.6) for a large negative dust energy density which results in a cyclic universe before inflation can possibly start. In each cycle, the Dirac observable of the volume of the universe increases very slightly. The cycles of the expansion and contraction continue for a long time as shown in the inset figure. The value of the Starobinsky field increases steadily in a step-like phenomena.

FIG. 6: This figure shows the characteristic evolution of the Dirac observable of the volume and the scalar field when inflation takes place after a few cycles of the expansion and contraction for the Starobinsky potential. The initial conditions are chosen as in (4.7) with a negative dust energy density. The volume in each cycle changes slightly which shows the hysteresis-like phenomena as discussed in [84].

hysteresis-like phenomena noted in effective dynamics in LQC in which the volume at the recollapse point grows in successive cycles [84] is found explicitly for this example.

IV.C. Klein-Gordon scalar field clocks

We now consider the case when a massless Klein-Gordon scalar field plays the role of a clock. For the standard kinetic energy, these clocks have positive energy density. In order to compare with the dust clocks which have positive energy density, we consider representative initial conditions in this case (at the bounce) at $O_V = 10^3$ as

$$O_{\rho_i} = -1.45, \quad O_{\rho_{\chi_i}} = 10^{-8},$$

(4.8)

here $O_{\rho_{\chi_i}}$ stands for the initial energy density of the massless Klein-Gordon scalar reference field which for comparison with solutions for dust clocks is set equal to the initial dust energy density in (4.3). With the initial values given in (4.8), one finds $O_{\pi_{\phi_i}} = \pm 900$. Similar to the cases in the
dust models, we choose positive $\mathcal{O}_{\pi_{\phi_i}}$ in our numerical analysis. Since the Dirac observable of the lapse is negative-valued in the Klein-Gordon scalar field model, we compensate this by choosing negative values for $\tau_{\chi}$ to study the evolution. As a result, when setting the bounce at $\tau_{\chi} = 0$, inflation takes place in the regime of negative values of $\tau_{\chi}$.

FIG. 7: In this figure, the initial conditions are chosen at the bounce with the initial values set by (4.8) for the Klein-Gordon scalar clock. In the left panel, we show the continuous evolution of the Dirac observable of the volume and the Hubble rate near the bounce while, in the right panel, we show the Dirac observable of the volume at late times until the inflationary phase. Also, in the right panel, the gray dashed vertical line marks the end of the superinflationary phase at $-\tau_{\chi} = 2.24 \times 10^{-5}$. The inflation takes place in the region beyond $-\tau_{\chi} = 3.81 \times 10^{-4}$ where the volume starts to increase rapidly. It ends quickly at $-\tau_{\chi} = 3.98 \times 10^{-4}$.

FIG. 8: With $\tau = 0$ at $\tau_{\chi} = 0$, the relation between $\tau$ and the Klein-Gordon scalar physical time is depicted from the bounce to the end of the inflation. As can be seen from the plot, $\tau_{\chi}$ changes only a little during inflation which starts at $\tau = 3.17 \times 10^9$.

In Fig. 7 we show the evolution of the Dirac observable of the volume and the Hubble rate near the bounce and the Dirac observable of the volume also at late times. In the figure, $\tau_{\chi} = 0$

\footnote{Note that in comparison with the unreduced LQC \cite{11} where Dirac quantization is applied, the Schrödinger equation involves a derivative with respect to the scalar field that is chosen as a clock. Because the Dirac observables are a power series in terms of $(\tau_{\chi} - \chi)$ a derivative of the observable with respect to $\tau_{\chi}$ and with respect to $\chi$ exactly differ by a minus sign which relates the $\tau_{\chi}$ used here to the physical time used in \cite{11}.}
corresponds to the bounce point, and the super-inflationary phase defined by the region when $\mathcal{O}_\rho = \rho_{\text{max}} \geq \mathcal{O}_\rho \geq \mathcal{O}_\rho = \rho_{\text{max}}/2$ ends at $\tau_\chi = -2.24 \times 10^{-5}$, yielding a total of 0.12 super-inflationary e-foldings. This phase then leads after a short time to slow roll inflation starting at $\tau_\chi = -3.81 \times 10^{-4}$ and ending at $\tau_\chi = -3.98 \times 10^{-4}$, yielding a total of 63.8 inflationary e-foldings.

In addition to the Klein-Gordon scalar field clock, we also plot the Dirac observable of the volume with respect to the dust time $\tau$, whose relation with $\tau_\chi$ is explicitly shown in Fig. [8]. Since the slope of the curve is inversely proportional to the volume, $\tau_\chi$ changes rather slowly during inflation. This explains why the inflation only lasts for a short period in the clock $\tau_\chi$. In Fig. [9] the Dirac observable of the volume and the slow-roll parameter is plotted with respect to $\tau$. In $\tau$ time, the superinflationary phase starts at $\tau = 0$ and ends at $\tau = 0.18$. Later, the inflation starts at $\tau = 3.17 \times 10^5$ and ends at $\tau = 5.52 \times 10^7$. Although the super-inflationary and inflationary phases start/end at different clock times as compared with the Klein-Gordon scalar field clock, the e-foldings of these two phases are the same in these clocks.

Note that the effects of the Klein-Gordon scalar reference field on the background dynamics are different from the dust reference field. This is due to the fact that the decay of the energy density of the Klein-Gordon scalar field is much faster than the dust energy density. As a result, even though we start with the same initial energy densities of the clock fields, the inflationary e-foldings in the two models turn out to be different. As discussed in section IV.A, for the initial conditions $4.3$, the inflationary e-folding with the dust clocks is 63.1, while the inflationary e-folding with the Klein-Gordon scalar clocks is 63.8 which is closer to the inflationary e-foldings, equal to $= 63.9$, without any reference clocks. As a result, starting from the same initial energy densities, the Klein-Gordon scalar reference field has less impact on the inflationary e-foldings than the dust reference field. Our numerical results also show that the effects of both clocks can be tuned as negligible as possible if the initial energy density of the clocks are set to small values. Finally, as in the case of dust reference fields there is an upper bound on the value of the energy density of the scalar reference field for inflation to occur. For initial conditions considered in the above example, this bound turns out to be 0.238 (in Planck units) which is much larger than the dust models.

As in the case of the dust models, we investigated the way a change in the initial energy density of the Klein-Gordon scalar field affects the duration of the pre-inflationary and inflationary phases. The results are shown in Fig. [10]. Note that starting with the same initial values of $\mathcal{O}_\phi$ in the parameter space, in the Klein-Gordon scalar field model, due to the faster decay of its energy density, the upper bound on the initial energy density of the Klein-Gordon scalar field is remarkably larger than that in the dust model. Due to this difference, the affect on e-foldings in the pre-inflationary and the inflationary regimes is different than for the dust models for the same initial conditions. For the dust model, shown in Fig. [2] when the initial dust energy density lies between $(10^{-7}, 10^{-4})$, we found a rapid decrease (increase) in the number of the inflationary (pre-inflationary) e-foldings while in the Klein-Gordon scalar field model, the decrease (increase) in the number of the inflationary (pre-inflationary) e-foldings becomes significant only when the initial energy density of the reference field grows above to 0.001 in Planck units. As a result, for the same initial values of $\mathcal{O}_\phi$ in the parameter space, the Klein-Gordon scalar reference field serves as a good clock in a larger part of the parameter space than the dust reference field. This phenomenological difference shows that dust and scalar reference clocks leave a distinct imprint in the inflationary dynamics.

Let us now summarize the main results of this section. Considering both the dust and Klein-Gordon scalar field clocks and assuming the validity of the effective dynamics, we found that the big bang singularity is resolved in the reduced phase space effective dynamics of LQC. Unlike the case of the positive dust energy density for which the universe is always in the expanding phase after the bounce, for the negative dust energy density this is not always the case. When the magnitude of the initial negative dust energy density exceeds an upper bound (determined by
FIG. 9: The evolution of the Dirac observable of the volume and the slow-roll parameter is depicted with respect to $\tau$ for the same initial conditions in Fig. 7. The vertical gray line stands for the onset of inflation which takes place at $t = 3.17 \times 10^5$. The inflation stops at $t = 5.52 \times 10^7$, yielding a total of 63.8 e-foldings which is close to the inflationary e-foldings without the reference fields. These plots show qualitative resemblance with Fig. 1 for the dust models.

FIG. 10: In the figure, we show the impact of the initial energy density of the Klein-Gordon scalar reference field on the pre-inflationary and the inflationary e-foldings when $O_{\phi_i} = -1.45$ and $O_{\pi_{\phi_i}} = 900$. Initially, the e-foldings change slowly with an increase in $O_{\rho\chi_i}$; it is only when $O_{\rho\chi_i} \gtrsim 0.001$, the e-foldings become more sensitively dependent on the initial values of the energy density of the Klein-Gordon scalar field.

initial conditions), the inflaton steadily rolls on the right wing of the potential and the universe enters into cycles of alternating expanding and contracting phases with a progressive change of the maximum volume at successive recollapse points. This phenomena can result in inflation to occur even after various cycles as we showed with another example. Though such a cyclic model is interesting, it does not correspond to ideal dust reference fields as such clocks should not change the qualitative dynamics of the background spacetime in such a significant way. When considering the case in which the inflaton is initially released from the left wing of the Starobinsky potential, we find although the dust clocks have a very limited impact on the pre-inflationary phase, it has some effect on the e-foldings of the slow-roll phase when the initial dust energy density becomes larger. Finally, when the massless Klein-Gordon scalar reference fields are considered as a clock, the universe evolves in a similar way as in the case of dust clocks with a positive energy density. The difference of the massless Klein-Gordon scalar clocks lies in the fact that starting with the same positive energy density, the massless Klein-Gordon scalar clock has less impact on the background dynamics than the dust clocks as the former decay much faster than the latter in an expanding
universe. From the numerical analysis, we find that the effects on inflation are not significant when the initial magnitude of the energy density of the clocks is much smaller than the energy density of the inflaton and both dust and Klein-Gordon scalar field clocks behave as good clocks in LQC for a large range of initial values. The effect on e-foldings in the different phases can be made as small as possible by decreasing the magnitude of the initial energy densities of the reference fields.

V. CONCLUSIONS

The goal of this paper is to understand the loop quantization of the spatially flat, homogeneous and isotropic FLRW universe sourced with an inflationary potential using reduced phase space quantization. We used the relational formalism with dust and Klein-Gordon scalar reference fields which act as clocks in the quantization procedure, obtained the basic structure of the quantum theory, showed that the resulting quantum gravitational Schrödinger equations are quantum difference equations which are non-singular and investigated some of the physical implications on bounce and inflationary dynamics in the effective spacetime description with the above clocks. The relational formalism has been used extensively in Dirac quantization of LQC but with a single massless scalar field as a clock [39–43, 45–48]. For the scalar field clock taken to be inflaton, the strategy successfully used in Dirac quantization in LQC [41] results in a time dependent evolution operator and the issue of the physical Hilbert space equipped with a conserved inner product becomes quite non-trivial. Further, the non-monotonic behavior of such a clock in the presence of inflationary potentials, only allows one to study a local patch near the classical singularity. A dust clock with as a single reference field has also been used employing techniques of LQC [30, 31]. However, in these treatments a detailed analysis of an inflationary potential was not included so far. Since in [30, 31] only a single reference field was considered, in contrast to four reference fields used in our analysis, it will be interesting to compare our work to the model in [30, 31] at the level of linear perturbations which will allow to distinguish aspects of Dirac versus reduced quantization in detail for the dust models. As far as the background dynamics is considered we can also extend the Dirac quantization in LQC [41] with inclusion of a scalar reference field which is not the inflaton. Here the classical starting point is the same as presented in our work for the Klein-Gordon scalar clock. Then we expect that via Dirac and reduced quantization the quantum gravitational Schrödinger equation to have the same form and the physical Hilbert space involve the same independent degrees of freedom. In our work we showed that various problems in the quantization procedure can be bypassed by introducing reference fields in addition to the inflaton field. In this work we considered three types of clocks: Brown-Kuchař and Gaussian dust clocks as well as the massless Klein-Gordon scalar field clock and studied a reduced phase quantization for a Starobinsky inflationary potential. The methods used in our analysis can be applied for any potential, including those for alternatives to inflation, and different quantum cosmological models.

The mini-superspace setting of LQC provides a finite dimensional framework in which the Gauss and spatial-diffeomorphism constraints are fixed at the classical level. The gravitational sector contributes two degrees of freedom to the reduced phase space, and another two arise from the inflaton field. We obtained the physical Hamiltonians in the reduced mini-superspace in terms of Dirac observables associated with these four degrees of freedom which are the Dirac observables of the connection and the conjugate triad as well as the inflaton and its conjugate momentum. We applied the improved dynamics or the $\bar{\mu}$ scheme in LQC to loop quantize the geometric degrees of freedom. As is usually the case in LQC, the inflaton field is quantized in the standard Schrödinger representation. The physical Hilbert space is spanned by the quantum states labeled by three parameters: the the volume of the universe, the value of the massive scalar field and the clock time. Using properties of the gravitational part of the Hamiltonian and the evolution operator
considered generally in LQC [76], the physical Hamiltonian in both of the cases turns out to be self-adjoint. We constructed the quantum theory in terms of operators corresponding to the Dirac observables and obtained the quantum dynamics using dust and Klein-Gordon scalar reference fields implemented on the physical Hilbert space. The evolution of physical states are governed by a Schrödinger-like quantum difference equation in which the action on $O_V$ is discrete while the action on $O_\phi$ is continuous. The quantum gravitational Schrödinger equations have a similar structure as the quantum difference equation in (Dirac quantized) LQC which have a uniform spacing in volume and are non-singular. For the reason that we can use the usual LQC representation for the physical Hilbert space in all three models the physical Hilbert space is still non-separable. However, as in (Dirac quantized) LQC, solutions of the quantum gravitational Schrödinger equation are expected to obey super-selection sectors and in this case if one restricts to the space of solutions of the quantum dynamics we expect that the space of solutions becomes a separable Hilbert space.

As a first step towards a better physical understanding of the dust and KG scalar field reference models we analyzed the dynamics in the reduced phase space with loop quantum corrections assuming the validity of the effective description of the quantum spacetime as is often assumed in LQC. Numerical simulations for various spacetimes show that for semi-classical states which are sharply peaked on a macroscopic universe at late times, the effective dynamics is an excellent approximation to the quantum difference evolution equation [41, 77, 79, 80]. Recently, attempts have been made to obtain effective dynamics in LQC from reduced phase space quantization of LQG using path-integral formulation with dust reference fields [36]. It will be interesting to investigate on these lines with inclusion of a potential and also with a Klein-Gordon scalar reference field. Using the above assumption for two-fluid models, we found the effective Hamiltonians in the reduced mini-superspace and derived the Hamilton’s equations and the modified Friedmann equations for dust and Klein-Gordon reference field models. As the Dirac observable of a function of the elementary phase space variables is just given by the function of the corresponding Dirac observables, the observable map is in this sense function preserving. Therefore, the modified Friedmann equations in the dust models take formally the same form as their counterpart in the standard LQC in cosmic time while the modified Friedmann equation in the Klein-Gordon scalar field model contains on its right hand side an additional multiplication factor proportional to the square of the Dirac observable of the lapse which is expected since the evolution is formulated with respect to the scalar field time and not the cosmic time. These modified equations effectively describe a dynamical system with two fluids coupled individually to the background spacetime. Besides, these two fluids, i.e. the massive scalar field and the clock field, satisfy their individual continuity equations and have no direct couplings between each other. From the modified Friedmann equations, we found that in the spatially flat FLRW universe of the reduced phase space, the big bang singularity is replaced with a quantum bounce which takes place at the maximum energy density $\rho_{\text{max}} \approx 0.41 \rho_{\text{Pl}}$ set by the quantum geometry.

To gain insights on the phenomenological implications of the clock fields, a numerical analysis was carried out based on the effective Hamilton’s equations. For the numerical analysis initial conditions were chosen at the bounce in a two-dimensional parameter space consisting of the scalar field $O_\phi$ and the energy density of the reference field which is a function of four elementary canonical variables in the reduced phase space. The initial conditions for the inflaton were given when the field starts rolling down in the left-wing of the potential (at the bounce). The field rolls up the right wing of the potential after the bounce, stops and then slow-rolls down yielding inflation. Depending on the sign and the magnitude of the dust energy density, different patterns of background dynamics are observed. For the positive dust energy, the presence of the dust field increases the Hubble friction, and thus decreases the duration of the inflationary phase for above initial conditions. Apart from inflation, the dust energy density can also slightly change the duration of the super-inflationary phase. On the other hand, for the negative dust energy, it has
opposite effects on the inflationary and super-inflationary phase. When the magnitude of the dust energy density does not exceed $\rho_{\text{upper}}$, increasing the magnitude of the negative dust energy density increases the inflationary e-foldings and at the same time slightly decreases the duration of the super-inflationary phase. However, when the magnitude of the negative dust energy density exceeds $\rho_{\text{upper}}$, the presence of the dust field significantly alters the qualitative dynamics of background spacetime. In this case, the total energy density becomes zero before the inflation sets in, causing a recollapse. The big crunch singularity of classical theory is resolved due to quantum geometric effects and the universe undergoes cycles of contracting and expanding phases. The volume of the universe grows slightly in successive cycles, leading to a change in the dust energy density between any two neighboring cycles. This reflects a mild hysteresis-like phenomena studied recently in LQC [84]. With the Starobinsky potential, while some initial conditions do not yield inflation even after long time, we showed existence of initial conditions which do lead to inflation after various cycles of contraction and expansion. In all the cases we find non-singular dynamics with dust clocks, in contrast to the classical theory where for the same inflationary potential the universe encounters the big bang singularity in past, and big crunch in future for sufficiently large negative dust energy density [65].

The effects of the Klein-Gordon scalar field clock turn out to be similar to the dust clock with a positive energy density. Starting from setting the initial conditions for the inflaton field in the left wing of the potential, we find following differences. First, the inflationary phase lasts for very short period in the time measured by the Klein-Gordon scalar field clock as compared with the dust clock. Secondly, since the energy density of the Klein-Gordon scalar field clock decays much faster than the dust clock, the former has less impact on the duration of inflation than the latter. By studying the impact of the initial energy density of the Klein-Gordon scalar field on the pre-inflationary and the inflationary phases, we find that with the same initial conditions in the parameter space, the number of the pre-inflationary and inflationary e-foldings in the Klein-Gordon scalar field model are quite different from those in the dust model. In particular, starting from the same initial energy density of the clock fields, the inflationary e-foldings in the Klein-Gordon scalar field model is larger than in the case of dust reference fields. In general, the Klein-Gordon scalar reference field serves as good clock in a larger subspace of the whole parameter space than the dust reference field with the positive energy density.

Apart from the inflationary e-foldings, we also find that with the same initial conditions in the parameter space, the e-foldings from the bounce to the moment when the pivot mode exits the horizon during inflation is also slightly different in the Klein-Gordon scalar field and the dust models. These e-foldings were found to be slightly larger for the dust reference fields. This implies the observable window of the primordial power spectrum for the quantum gravitational effects are also changed when different physical times are employed if we choose the same initial conditions for different reference field models. Note that even though, the Gaussian and Brown-Kuchař dust models have exactly the same background dynamics in the spatially flat FLRW universe, from the analysis in [65], a difference in the scalar power spectrum is still expected as the equations of motion for the linear perturbations are different in the two dust models. It will be interesting to generalize the latter analysis to LQC and explore the consequences of choosing different dust and scalar clocks on the primordial power spectrum in detail. While above results indicate that starting from same initial conditions for clock densities, different reference fields can leave tiny but distinct imprints on inflationary dynamics, one can of course choose different initial conditions for different clocks to get same phenomenological effects. In this sense, the multiple choice problem of time, which leaves traces in phenomenology, is linked with the problem of initial conditions. Finally, one can always choose initial conditions for the clock densities such that their contribution to observational quantities is less than the experimental error.

In summary, we applied a reduced phase space quantization to the two-fluid dust models and the
Klein-Gordon scalar field model for a spatially flat FLRW universe with an inflationary potential, where the geometric degrees of freedom were loop quantized. As a first step towards a better physical understanding of these models we also studied the effective Hamilton’s equations and the modified Friedmann equations in these three reference field models. The evolution of the universe in the dust and Klein-Gordon reference field models is qualitatively similar to that in (Dirac quantized) LQC as long as the energy density of the inflaton is dominant at all times. In particular, we found that the slow-roll inflation take place when the dust and Klein-Gordon scalar fields serve as good clocks with energy densities much smaller than that of the inflaton field.

A more detailed understanding of these models can be obtained by investigating the physical solutions, and quantum dynamics directly. Compared to the current models in LQC the already existing numerical techniques need to be generalized to the two-fluid case. Due to the presence of a reference field independent of the potential, this is computationally more involved than numerical simulations done so far in isotropic (Dirac quantized) LQC [41, 80]. The situation is closer to anisotropic models which have more degrees of freedom. Given that the latter have been successfully analyzed in detail using super-computing methods [77, 79], the numerical infrastructure can be adapted to study quantum dynamics in reduced phase space quantization. Apart from the question of singularity resolution at the level of physical Hilbert space, this step is important since it will allow to test the validity of effective techniques for two-fluid models. Further, it opens the possibility to better compare to for instance the model in [39, 41] at the quantum level, always taking into account that we compare models with different degrees of freedom in the physical Hilbert space. A long term future project will be, once the quantum background dynamics is well understood, to consider linear perturbations which opens a window to further analyze the different features of the dust and Klein-Gordon scalar fields models. For instance the fact that the physical Hamiltonians in the two dust models coincide is only a special property of the FLRW spacetime and no longer holds if perturbations are taken into account. An analysis on above lines would provide a consistent and complete quantum gravitational treatment of inflationary spacetimes where the role of clocks in the background dynamics as well as in perturbations, and important issues such as the physical Hilbert space and the conserved inner product in presence of an inflationary potential, and resulting impacts on phenomenology will be settled.

Acknowledgements

This work is supported by the DFG-NSF grants PHY-1912274 and 425333893 and NSF grant PHY-1454832. K.G. thanks the LSU gravity group for their kind hospitality during a visit where part of this work was done.

[1] K. V. Kuchar, Time and interpretations of quantum gravity, Int. J. Mod. Phys. D20, 3 (2011).
[2] A. Ashtekar, J. Lewandowski, D. Marolf, J. Mourao, and T. Thiemann, Quantization of diffeomorphism invariant theories of connections with local degrees of freedom, J. Math. Phys. 36, 6456 (1995), arXiv:gr-qc/9504018.
[3] A. Ashtekar and P. Singh, Loop Quantum Cosmology: A Status Report, Class. Quant. Grav. 28, 213001 (2011), arXiv:1108.0893.
[4] P. G. Bergmann, ‘Gauge-Invariant’ Variables in General Relativity, Phys. Rev. 124, 274 (1961).
[5] P. G. Bergmann, Observables in General Relativity, Rev. Mod. Phys. 33, 510 (1961).
[6] A. Komar, Construction of a Complete Set of Independent Observables in the General Theory of Relativity, Phys. Rev. 111, 1182 (1958).
[7] C. Isham, Canonical quantum gravity and the problem of time, NATO Sci. Ser. C 409, 157 (1993), arXiv:gr-qc/9210011
[8] E. Anderson, The Problem of Time in Quantum Gravity, (2010), arXiv:1009.2157.
[9] C. Rovelli, What Is Observable in Classical and Quantum Gravity?, Class. Quant. Grav. 8, 297 (1991).
[10] C. Rovelli, Partial observables, Phys. Rev. D65, 124013 (2002), arXiv:gr-qc/0110035.
[11] A. S. Vytheeswaran, Gauge unfixing in second class constrained systems, Annals Phys. 236, 297 (1994).
[12] B. Dittrich, Partial and complete observables for Hamiltonian constrained systems, Gen. Rel. Grav. 39, 1891 (2007), arXiv:gr-qc/0411013.
[13] B. Dittrich, Partial and complete observables for canonical general relativity, Class. Quant. Grav. 23, 6155 (2006), arXiv:gr-qc/0507106.
[14] T. Thiemann, Reduced phase space quantization and Dirac observables, Class. Quant. Grav. 23, 1163 (2006), arXiv:gr-qc/0411031.
[15] J. Pons, D. Salisbury, and K. Sundermeyer, Revisiting observables in generally covariant theories in the light of gauge fixing methods, Phys. Rev. D 80, 084015 (2009), arXiv:0905.4564.
[16] J. Pons, D. Salisbury, and K. Sundermeyer, Observables in classical canonical gravity: folklore demystified, J. Phys. Conf. Ser. 222, 012018 (2010), arXiv:1001.2726.
[17] B. Dittrich and J. Tambornino, A Perturbative approach to Dirac observables and their space-time algebra, Class. Quant. Grav. 24, 757 (2007), arXiv:gr-qc/0610060.
[18] K. Giesel, S. Hofmann, T. Thiemann, and O. Winkler, Manifestly Gauge-Invariant General Relativistic Perturbation Theory. I. Foundations, Class. Quant. Grav. 27, 055005 (2010), arXiv:0711.0115.
[19] K. Giesel, S. Hofmann, T. Thiemann, and O. Winkler, Manifestly Gauge-invariant general relativistic perturbation theory. II. FRW background and first order, Class. Quant. Grav. 27, 055006 (2010), arXiv:0711.0117.
[20] K. Giesel and T. Thiemann, Scalar Material Reference Systems and Loop Quantum Gravity, Class. Quant. Grav. 32, 135015 (2015), arXiv:1206.3807.
[21] M. Ali, V. Husain, S. Rahmati, and J. Ziprick, Linearized gravity with matter time, Class. Quant. Grav. 33, 105012 (2016), arXiv:1512.07854.
[22] K. Giesel and A. Herzog, Gauge invariant canonical cosmological perturbation theory with geometrical clocks in extended phase-space A review and applications, Int. J. Mod. Phys. D27, 1830005 (2018), arXiv:1712.09878.
[23] K. Giesel, A. Herzog, and P. Singh, Gauge invariant variables for cosmological perturbation theory using geometrical clocks, Class. Quant. Grav. 35, 155012 (2018), arXiv:1801.08630.
[24] K. Giesel, P. Singh, and D. Winneken, Dynamics of Dirac observables in canonical cosmological perturbation theory, Class. Quant. Grav. 36, 085009 (2019), arXiv:1811.07972.
[25] L. Herold, Cosmological perturbation theory with Gaussian dust reference fields, Master thesis, FAU Erlangen-Nürnberg (2019).
[26] Y. Han, K. Giesel, and Y. Ma, Manifestly gauge invariant perturbations of scalar-tensor theories of gravity, Class. Quant. Grav. 32, 135006 (2015), arXiv:1501.04947.
[27] K. Giesel, J. Tambornino, and T. Thiemann, LTB spacetimes in terms of Dirac observables, Class. Quant. Grav. 27, 105013 (2010), arXiv:0906.0569.
[28] K. Giesel and T. Thiemann, Algebraic quantum gravity (AQG). IV. Reduced phase space quantisation of loop quantum gravity, Class. Quant. Grav. 27, 175009 (2010), arXiv:0711.0119.
[29] M. Domagala, K. Giesel, W. Kaminski, and J. Lewandowski, Gravity quantized: Loop Quantum Gravity with a Scalar Field, Phys. Rev. D82, 104038 (2010), arXiv:1009.2445.
[30] V. Husain and T. Pawlowski, Dust reference frame in quantum cosmology, Class. Quant. Grav. 28, 225014 (2011), arXiv:1108.1147.
[31] V. Husain and T. Pawlowski, Time and a physical Hamiltonian for quantum gravity, Phys. Rev. Lett. 108, 141301 (2012), arXiv:1108.1145.
[32] K. Giesel and A. Vetter, Reduced loop quantization with four Klein Gordon scalar fields as reference matter, Class. Quant. Grav. 36, 145002 (2019), arXiv:1610.07422.
[33] K. Giesel and A. Oelmann, Comparison Between Dirac and Reduced Quantization in LQG-Models with Klein-Gordon Scalar Fields, Acta Phys. Polon. Supp. 10, 339 (2017).
[34] M. Ali, S. M. Hassan, and V. Husain, Universe as an oscillator, Phys. Rev. D98, 086002 (2018), arXiv:1807.03864.
quantum gravity, Phys. Rev. D 96, 024043 (2017), arXiv:1702.01688.

[63] K. V. Kuchar and C. G. Torre, Gaussian reference fluid and interpretation of quantum geometrodynamics, Phys. Rev. D 43, 419 (1991).

[64] J. D. Brown and K. V. Kuchar, Dust as a standard of space and time in canonical quantum gravity, Phys. Rev. D 51, 5600 (1995), arXiv:gr-qc/9409001.

[65] K. Giesel, L. Herold, B.-F. Li, and P. Singh, Mukhanov-Sasaki equation in manifestly gauge-invariant linearized cosmological perturbation theory with dust reference fields, To appear in Phys. Rev. D., arXiv:1912.11490.

[66] T. Thiemann, Solving the Problem of Time in General Relativity and Cosmology with Phantoms and k-Essence, (2006), arXiv:astro-ph/0607380.

[67] K. Giesel, Introduction to Dirac observables, Int. J. Mod. Phys. A23, 1190 (2008).

[68] A. Corichi and P. Singh, Is loop quantization in cosmology unique?, Phys. Rev. D 78, 024034 (2008), arXiv:0805.0136.

[69] M. Martin-Benito, G. A. Marugan, and J. Olmedo, Further Improvements in the Understanding of Isotropic Loop Quantum Cosmology, Phys. Rev. D 80, 104015 (2009), arXiv:0909.2829.

[70] K. Liegener and P. Singh, New Loop Quantum Cosmology Modifications from Gauge-covariant Fluxes, arXiv:gr-qc/1908.07001.

[71] J. Lewandowski, A. Okolow, H. Sahlmann, and T. Thiemann, Uniqueness of diffeomorphism invariant states on holonomy-flux algebras, Commun. Math. Phys. 267, 703 (2006), arXiv:gr-qc/0504147.

[72] C. Fleischhack, Representations of the Weyl algebra in quantum geometry, Commun. Math. Phys. 285, 67 (2009), arXiv:math-ph/0407006.

[73] A. Ashtekar and M. Campiglia, On the Uniqueness of Kinematics of Loop Quantum Cosmology, Class. Quant. Grav. 29, 242001 (2012), arXiv:1209.4374.

[74] J. Engle, M. Hanusch, and T. Thiemann, Uniqueness of the Representation in Homogeneous Isotropic LQC, Commun. Math. Phys. 354, 231 (2017), arXiv:1609.03548 [Erratum: Commun.Math.Phys. 362, 759-760 (2018)].

[75] T. Thiemann, Quantum spin dynamics (QSD), Class. Quant. Grav. 15, 839 (1996), arXiv:9606089.

[76] W. Kaminski, J. Lewandowski, and T. Pawlowski, Physical time and other conceptual issues of QG on the example of LQC, Class. Quant. Grav. 26, 035012 (2009), arXiv:0809.2590.

[77] P. Singh, Glimpses of space-time beyond the singularities using supercomputers, arXiv:1809.01747.

[78] P. Diener, B. Gupt, and P. Singh, Chimera: A hybrid approach to numerical loop quantum cosmology, Class. Quant. Grav. 31, 025013 (2014), arXiv:1310.4795.

[79] P. Diener, A. Joe, M. Megavand, and P. Singh, Numerical simulations of loop quantum Bianchi-I spacetimes, Class. Quant. Grav. 34, 094004 (2017), arXiv:1701.05824.

[80] P. Diener, B. Gupt, and P. Singh, Numerical simulations of a loop quantum cosmos: robustness of the quantum bounce and the validity of effective dynamics, Class. Quant. Grav. 31, 105015 (2014), arXiv:1402.6613.

[81] V. Taveras, Corrections to the Friedmann Equations from LQG for a Universe with a Free Scalar Field, Phys. Rev. D 78, 064072 (2008), arXiv:0807.3325.

[82] G. J. Olmo and P. Singh, Covariant effective action for loop quantum cosmology a la Palatini, JCAP 0901:030, arXiv:0806.2783.

[83] B.-F. Li, P. Singh, and A. Wang, Genericity of pre-inflationary dynamics and probability of the desired slow-roll inflation in modified loop quantum cosmologies, Phys. Rev. D100, 063513 (2019), arXiv:1906.01004.

[84] J. L. Dupuy and P. Singh, Hysteresis and beating phenomena in loop quantum cosmology, Phys. Rev. D 101, 086016 (2020), arXiv:1912.11490.