Ambiguous power spectrum from a quantum bounce

Jaime de Cabo Martin,[1,*] Przemysław Małkiewicz,[1,†] and Patrick Peter[2,3,‡]

[1]*National Centre for Nuclear Research, Pasteura 7, 02-093 Warszawa, Poland*
[2]*GReCO—Institut d'Astrophysique de Paris, CNRS and Sorbonne Université, UMR 7095 98 bis boulevard Arago, 75014 Paris, France*
[3]*Centre for Theoretical Cosmology, Department of Applied Mathematics and Theoretical Physics, University of Cambridge, Wilberforce Road, Cambridge CB3 0WA, United Kingdom*

(Received 2 January 2023; accepted 9 February 2024; published 12 March 2024)

A quantum cosmological bouncing model may exhibit an ambiguity stemming from the nonclassical nature of the background evolution: Two classically equivalent theories can produce two qualitatively different potentials sourcing the perturbations. It reflects the general ambiguity in quantization of the gravitational field at linear order. We derive explicitly the quantum canonical transformation of linear perturbations involving the quantum background to show how it leads to inequivalent theories. We identify the relevant quantum parameter describing the difference and expand upon the ambiguity by calculating the expected power spectra produced for initial quantum vacuum fluctuations in the contracting phase of both potentials. We find that one spectral index corresponds to all values of this parameter but one, while the other thus represents a set of measure zero.

DOI: 10.1103/PhysRevD.109.066009

I. INTRODUCTION

In a previous work [1], we studied a cosmological model whose dynamics is led by general relativity (GR) and a perfect fluid with arbitrary equation of state. Classically, the solutions either contract toward or expand from a singularity: Quantization permits one to regularize the trajectories (dubbed "semiquantum" in [1]), thereby leading to a quantum bouncing behaviour.

Quantization of a cosmological model replaces the four-dimensional spacetime with what we shall call a "quantum spacetime" that violates the properties of classical geometry. For instance, the dynamical law for a field in a classical spacetime can be formulated in terms of different field variables. In the Hamiltonian formalism used in this work, these variables are connected by canonical transformations. The fact that they all undergo physically equivalent evolutions can be viewed as a manifestation of a unique underlying background spacetime that imposes a unique dynamical law on the field. In passing to quantum theory of the background spacetime, on the other hand, the use of different field variables may result in their very different quantum dynamics. It is so because the field no longer propagates in a fixed spacetime but rather in a "quantum spacetime," and the physical discrepancies between the evolutions of different field variables reflect the "quantumness of spacetime." As found in Ref. [1], simple rescalings of the curvature perturbation in a quantum Friedmann universe by powers of the scale factor produce different gravitational potentials in the Mukhanov-Sasaki equation, thereby making the dynamics of the perturbation depend on the choice of the field variable employed in its quantization.

In the present work, we study the physical consequences of the ambiguity in the dynamical law for the scalar perturbation due to quantization of the background spacetime. If the infinitely many gravitational potentials found in [1] actually correspond to infinitely many physical predictions, then the theory is to be considered unphysical. Currently, the literature (see, e.g., [2–5]) provides only one solution to the primordial power spectrum from a quantum bounce. We note that the simplest known quantum bounces produce only blue-tilted power spectrum contrary not only to inflationary predictions but also to observations; finding new solutions could improve this situation.

Our work also pertains to the question of the usefulness of the Mukhanov variable for describing scalar perturbations in a quantum universe. In inflationary models based on classical backgrounds, it is convenient to use the Mukhanov variable because it allows one to asymptotically define a quantum vacuum in the same way as for flat spacetime. However, it is not the only valid choice for the perturbation variables even in the context of inflation as discussed, e.g., in Ref. [6]. In a fully quantum universe, the issue is even less clear as the choice of perturbation variables can influence both the definition of the initial

*jaimedk6.95@gmail.com
†Przemyslaw.Malkiewicz@ncbj.gov.pl
‡peter@iap.fr

vacuum state and the dynamics of perturbations. Thus, in the context of our work, it is natural to ask whether the Mukhanov variable remains a preferred choice in a fuller, more quantum description of the primordial Universe or if it should be replaced with another, better-suited, variable. The latter situation would not be exceptional as there exist situations for which the Mukhanov variable may become singular and other variables, such as the Bardeen potential, must be used instead.

The problem of choosing the fundamental variables for passing to quantum theory is related to the factor-ordering problem. Both issues arise from the absence of a canonical isomorphism between the Poisson algebra of phase space observables and the quantum operator algebra. A canonical isomorphism is only feasible for a very limited set of observables, such as the fundamental observables in canonical quantization: momentum, position, and their quadratic functions (see, e.g., Ref. [7]). Consequently, the choice of fundamental observables typically influences the resulting quantum theory.

The factor-ordering problem appears on top of this choice and applies to most of the compound observables. Proposed fundamental gravitational variables include the Arnowitt-Deser-Misner (ADM) or Ashtekar variables [8], each formulation suffering from its own factor-ordering problem (see, e.g., [9,10]). In the former formulation, a possible resolution to the factor-ordering problem with the Hamiltonian constraint could involve insisting on its covariance with respect to coordinate transformations on the ADM configuration space [11]; this procedure applies in a straightforward way if the Hamiltonian happens to be quadratic in the momenta. Alternatively, one might demand that, after quantization, the constraints remain first-class[1] [12,13]. Notably, these proposals might not have a unique solution regarding factor ordering [14]. The ambiguity is further magnified when finding the kernel of the constraint operators is accompanied by promoting one of the variables to an internal time variable and redefining the scalar product in the Hilbert space to achieve a dynamical interpretation of the theory [15].

Additionally, instead of quantizing the full ADM phase space, one may prefer to first solve the constraints of the classical theory by removing unphysical degrees of freedom and choosing some internal "spacetime" variables with respect to which the spatial and temporal dependence of the physical fields would be expressed [15]. In this approach, only physical variables are quantized. The issue of preferred fundamental physical variables, not to mention factor ordering, seems to be rather hopeless as seen in cosmological perturbation theory, notorious for its ambiguous gauges and gauge-invariant variables. This is the specific case addressed in this paper. We believe that the ambiguity explored here is universal, reflecting the general ambiguity in quantization of the gravitational field at the linear perturbation level.

As the last point of this introduction, let us remark that we view our framework of quantum fields in quantum spacetime as a truncation of a full theory of quantum gravity. The dynamics in the latter would naturally be expressed in some internal time variable. Even if many internal time variables are available, the particular choice one makes does not seem to be crucial for the physical predictions of quantum gravity (we refer the interested reader to some of our previous works devoted to this issue [16–20]). Nevertheless, if a truncation is to be consistent, it should make use of a unique internal time variable for quantizing and describing all dynamical variables, both for the background and the perturbations. We emphasize that our framework satisfies this requirement.

The plan of this work is as follows. In Sec. II, we introduce our cosmological model: We first define the classical model with a special attention paid to the definition of perturbation variables, and then we quantize it and set up its semiclassical approximation. We next identify and discuss the dynamical ambiguity in the resulting quantum model. In Secs. III and IV, we study the ambiguity in detail: We solve the dynamical equations and find all the possible physical predictions for the amplitude and the spectral index of primordial perturbations, which could be derived from the model. We find that there are only two types of predictions that can be produced by quantum bounce models. Section V gathers our conclusions.

II. THE AMBIGUITY

Before going on to the new results obtained in this work, let us summarize the framework of the semiquantum ambiguity.

A. Background dynamics

We begin by defining the model used throughout. We expand our spacetime manifold $\mathcal{M}$ as $\mathcal{M} \simeq \mathbb{R} \times \mathbb{T}^3$, whose background metric is given by the isotropic and homogeneous flat Friedmann-Lemaître-Robertson-Walker (FLRW) metric

$$\mathrm{d}s^2 = -N^2(\tau)\mathrm{d}\tau^2 + a^2(\tau)\gamma_{ij}\mathrm{d}x^i\mathrm{d}x^j, \tag{1}$$

in units in which the velocity of light is $c = 1$. We assume that the spatial part is compact with coordinate volume

$$\mathcal{V}_0 \coloneqq \int \sqrt{\gamma}\mathrm{d}^3x, \tag{2}$$

while the scale factor $a(\tau)$ has its dynamics driven by GR sourced by a perfect fluid with constant equation of state parameter $0 < w = p/\rho < 1$ (with p the pressure and ρ the

[1]These proposals are related but not identical.

energy density). The overall Einstein-Hilbert-Schutz action then reads [21,22]

$$\mathcal{S}_{\rm EHS} = \frac{1}{2\kappa}\int \mathrm{d}^4x\sqrt{-g}R + \int \mathrm{d}^4x\sqrt{-g}P(w,\phi), \quad (3)$$

where $\kappa = 8\pi G_{\rm N}$, and ϕ defines the cosmic fluid flow. We use the expansion of this action to second order and an adaptation of the fully canonical formalism from [23] so as to obtain a Hamiltonian description in which only the truly physical degrees of freedom are considered.

1. Classical dynamics

Setting the lapse function to $N = (1+w)a^{3w}$, the fluid part of the action contributes a linear momentum term to the Hamiltonian [24], so the fluid merely serves as a clock in what follows. Going from $\{a, p_a\}$ to $\{q, p\}$, defined by

$$q = \frac{4\sqrt{6}}{3(1-w)\sqrt{1+w}}a^{\frac{3}{2}(1-w)} \equiv \gamma a^{\frac{3}{2}(1-w)}, \quad (4)$$

and

$$p = \frac{\sqrt{6(1+w)}}{2\kappa_0}a^{\frac{3}{2}(1+w)}H, \quad (5)$$

with $H = \dot{a}/(Na)$ the Hubble rate and $\kappa_0 = \kappa/\mathcal{V}_0$, the zeroth-order gravitational Hamiltonian reads

$$H^{(0)} = 2\kappa_0 p^2, \quad (6)$$

where we reverted the direction of time with respect to the fluid variable to make it positive. We hereafter use τ as internal clock, assuming it coincides with the FLRW time set in (1).

The solutions of the equations of motion stemming from (6) read

$$q_{\rm cl}(\tau) = 4\sqrt{2\kappa_0 H^{(0)}}(\tau-\tau_{\rm s}) \quad \text{and} \quad p_{\rm cl}(\tau) = \sqrt{\frac{H^{(0)}}{2\kappa_0}}, \quad (7)$$

where $H^{(0)}$ is a constant. These classical trajectories either terminate at or emerge from the singularity $q \to 0$ (and thus $a \to 0$) at time $\tau_{\rm s}$. They are straight lines in phase space $\{q, p\}$ with constant p [16].

2. Quantum dynamics

Quantization of (6) is not as trivial as it seems. Of course, one can merely impose a canonical rule and straightforwardly set $p \mapsto \hat{P} = -i\hbar\partial/\partial q$, but it turns out that $\hat{P}$ is not a self-adjoint operator and cannot serve as a fundamental variable. A more justified approach involves defining the self-adjoint dilation operator $qp \mapsto \hat{D} = \frac{1}{2}(\hat{Q}\hat{P} + \hat{P}\hat{Q})$ as a fundamental variable alongside the position operator. The canonical commutation rule is then recast as $[\hat{Q}, \hat{D}] = i\hat{Q}$. This introduces the factor-ordering problem for (6) as $p^2 \mapsto$ "any combination of $\hat{Q}$ and $\hat{D}$ classically equivalent to $\hat{Q}^{-2}\hat{D}^2$." In Ref. [19], it was determined that for a broad class of orderings, one obtains

$$H^{(0)} \mapsto \hat{H}^{(0)} = 2\kappa_0\big(\hat{P}^2 + \mathfrak{c}_0\hat{Q}^{-2}\big), \quad (8)$$

where the parameter $\mathfrak{c}_0 \geq 0$ depends on the specific ordering.

The self-adjoint operators $\hat{Q}$ and $\hat{D}$ generate a unitary group of affine transformations applicable for covariant integral quantizations of the half-plane (q, p)—analogous to the role played by the Weyl-Heisenberg group (based on $\hat{Q}$ and $\hat{P}$) in quantizations of the full plane, including Weyl (canonical) quantization [24]. This approach, termed "affine quantization," not only confirms the result (8) but also provides a means of parametrizing the factor-ordering ambiguity. For generality, we leave $\mathfrak{c}_0$ unspecified, emphasizing that all choices of $\mathfrak{c}_0 \geq 0$ yield the same qualitative dynamics of the Universe rebounding against the singularity $q = 0$. For $\mathfrak{c}_0 = 0$, one recovers the canonical case, while for $\mathfrak{c}_0 \geq \frac{3}{4}\hbar^2$, the Hamiltonian $\hat{H}^{(0)}$ becomes essentially self-adjoint, and no boundary condition is required at $q = 0$ to ensure a unique and unitary dynamics.

A useful approximate semiclassical (or, rather, semiquantum [1]) solution is obtained with a family of coherent states [25] built upon a so-called fiducial state $|\xi\rangle$, satisfying $\langle\xi|\hat{Q}|\xi\rangle = 1$ and $\langle\xi|\hat{P}|\xi\rangle = 0$, namely

$$|q(\tau), p(\tau)\rangle = \mathrm{e}^{ip(\tau)\hat{Q}/\hbar}\mathrm{e}^{-i\ln q(\tau)\hat{D}/\hbar}|\xi\rangle. \quad (9)$$

These states, written in short $|q, p\rangle$ when there is no risk of confusion, are such that the expectation values of $\hat{P}$ and $\hat{Q}$ are, respectively, $\langle q, p|\hat{Q}|q, p\rangle = q(\tau)$ and $\langle q, p|\hat{P}|q, p\rangle = p(\tau)$.

Setting

$$H_{\rm sem} = \langle q, p|\hat{H}^{(0)}|q, p\rangle = 2\kappa_0\left(p^2 + \frac{\mathfrak{K}}{q^2}\right), \quad (10)$$

with $\mathfrak{K} > 0$ a constant depending on the family of coherent states chosen for the semiquantum approximation, it can be shown that $q(\tau)$ and $p(\tau)$ satisfy the Hamilton equations derived from $H_{\rm sem}$, with solutions

$$q = q_{\rm B}\sqrt{1+(\omega\tau)^2}, \quad (11a)$$

$$p = \frac{q_{\rm B}\omega^2}{4\kappa_0}\frac{\tau}{\sqrt{1+(\omega\tau)^2}}, \quad (11b)$$

where $q_{\rm B}^2 = 2\kappa_0 \mathfrak{K}/H_{\rm sem}$ and $\omega^2 = 4H_{\rm sem}^2/\mathfrak{K}$. The singularity is clearly replaced by a bouncing behaviour, as expected.

B. Perturbations

Compactness of space implies discrete Fourier wave vectors $\boldsymbol{k}$, and the second-order Hamiltonian $H^{(2)}$ is naturally a sum over independent contributions $H_{\boldsymbol{k}}^{(2)}$ for each mode. The relevant perturbation variables, noted $\phi_{\boldsymbol{k}}$ in what follows, are obtained as a combination of the fluid variable $\delta\phi_{\boldsymbol{k}}$ and the intrinsic curvature perturbation $\delta R_{\boldsymbol{k}}$, namely

$$\begin{aligned}\phi_{\boldsymbol{k}} &= \frac{1}{\sqrt{2\kappa_0}\mathcal{V}_0}\left[\frac{\bar{p}^\phi \delta\phi_{\boldsymbol{k}}}{\sqrt{w(1+w)}p} + \sqrt{\frac{6}{w}}a^{\frac{3}{2}(1-w)}\frac{a^2}{4\mathcal{V}_0^{2/3}k^2}\delta R_{\boldsymbol{k}}\right],\\ \pi_{\phi,\boldsymbol{k}} &= \sqrt{2\kappa_0}\left[\sqrt{w(1+w)}\frac{a^{3(1+w)}p}{|\bar{p}^\phi|^{1+w}}\delta\rho_{\boldsymbol{k}} - \frac{3(1-w)a^2 p}{8\mathcal{V}_0^{2/3}k^2}\right.\\ &\quad\left.\times\sqrt{\frac{1+w}{w}}\delta R_{\boldsymbol{k}} - \sqrt{\frac{3}{8w}}(1+w)a^{-\frac{3}{2}(1-w)}\bar{p}^\phi\delta\phi_{\boldsymbol{k}}\right], \quad (12)\end{aligned}$$

where $\delta\rho_{\boldsymbol{k}}$ represents the fluid energy density perturbation, while the background variable $\bar{\phi}$ and its momentum $\bar{p}^\phi$ describe the fluid, with $-i\boldsymbol{k}\bar{p}^\phi\delta\phi_{\boldsymbol{k}}$ defining the flow of the fluid energy through the surface orthogonal to $\boldsymbol{k}$ (see details in Ref. [23]).

In term of the above variables, the Hamiltonian reads

$$H_{\boldsymbol{k}}^{(2)} = \frac{1}{2}\left[|\pi_{\phi,\boldsymbol{k}}|^2 + w(1+w)^2\left(\frac{q}{\gamma}\right)^{4r_{\rm F}}k^2|\phi_{\boldsymbol{k}}|^2\right], \quad (13)$$

with

$$r_{\rm F} = -\frac{1-3w}{3(1-w)}, \quad (14)$$

whose numerical value lies in the range $-\frac{1}{3} \le r_{\rm F} \le 0$ for the range of equation of state $0 \le w \le \frac{1}{3}$ we are concerned with.

Curvature perturbations, which are observationally relevant gauge-invariant variables, can be easily derived from (12). They are often calculated on comoving hypersurfaces, thereby defining $\mathcal{R}_{\boldsymbol{k}}$ through $a^2k^2\mathcal{R}_{\boldsymbol{k}} = -4\delta R_{\boldsymbol{k}}|_{\delta\phi=0}$ (with a conventional minus sign), reading

$$\mathcal{R}_{\boldsymbol{k}} = -\sqrt{\frac{w\kappa_0}{3}}a^{-\frac{3}{2}(1-w)}\phi_{\boldsymbol{k}}, \quad (15)$$

or uniform-density hypersurfaces ($\zeta_{\boldsymbol{k}}$), i.e. $a^2k^2\zeta_{\boldsymbol{k}} = 4\delta R_{\boldsymbol{k}}|_{\delta\rho=0}$, which is

$$\zeta_{\boldsymbol{k}} = \frac{\mathcal{V}_0}{2}\sqrt{\frac{\kappa_0}{3w}}\frac{(1+w)\phi_{\boldsymbol{k}}}{a^{\frac{1}{2}(1-w)}} + \frac{\pi_{\phi,\boldsymbol{k}}}{3p\sqrt{2w(1+w)\kappa_0}}. \quad (16)$$

Note that it is usually assumed, e.g., using initial conditions for the expanding Universe at the end of inflation, that $\phi_{\boldsymbol{k}} \gg \pi_{\phi,\boldsymbol{k}}$, leaving only the first term.

The classical theory based on the Hamiltonian (13) can be written using a different set of variables by performing a time-dependent canonical transformation. Let us define new variables via the rescaling

$$v_{\boldsymbol{k}} = Z\phi_{\boldsymbol{k}} \quad \text{and} \quad \pi_{v,\boldsymbol{k}} = Z^{-1}\pi_{\phi,\boldsymbol{k}} + \frac{\dot{Z}}{Z^2}\phi_{\boldsymbol{k}}, \quad (17)$$

where Z is any nonvanishing phase space function. This transforms the Hamiltonian into

$$H_{\boldsymbol{k}}^{(2)} = \frac{1}{2}Z^2\left\{|\pi_{v,\boldsymbol{k}}|^2 + \left[\frac{w(1+w)^2}{Z^4}\left(\frac{q}{\gamma}\right)^{4r_{\rm F}}k^2 - \mathcal{V}\right]|v_{\boldsymbol{k}}|^2\right\}, \quad (18)$$

where the potential $\mathcal{V}$ is defined through

$$\mathcal{V} = \frac{1}{Z^4}\left[\frac{\ddot{Z}}{Z} - 2\left(\frac{\dot{Z}}{Z}\right)^2\right]. \quad (19)$$

An interesting and useful one-parameter family of such scale transformations is obtained by setting

$$Z_r = \sqrt{1+w}\left(\frac{q}{\gamma}\right)^r, \quad (20)$$

which yields

$$H_{\boldsymbol{k}}^{(2)} = \frac{1+w}{2}\left(\frac{q}{\gamma}\right)^{2r}\left(|\pi_{v,\boldsymbol{k}}|^2 + \Omega_r^2|v_{\boldsymbol{k}}|^2\right), \quad (21)$$

with

$$\Omega_r^2 = \left(\frac{q}{\gamma}\right)^{4(r_{\rm F}-r)}wk^2 + \frac{r(r+1)(4\kappa_0)^2}{q^2(1+w)^2}\left(\frac{q}{\gamma}\right)^{-4r}p^2, \quad (22)$$

where we used the classical solution (7). It should be noted at this point that setting $r = r_{\rm F}$ and introducing the conformal time η through

$$\mathrm{d}\eta = (1+w)\left(\frac{q}{\gamma}\right)^{2r_{\rm F}}\mathrm{d}\tau = Z_{r_{\rm F}}^2\mathrm{d}\tau \quad (23)$$

removes the overall coefficient in front of the Hamiltonian (21), turning the kinetic term into its canonical form, while (22) takes the simple and usual form

$$\Omega_{r_{\rm F}}^2 = wk^2 - \frac{Z_{r_{\rm F}}''}{Z_{r_{\rm F}}},$$

where a prime means a derivative with respect to the conformal time η. The variable $v_{\boldsymbol{k}}$ in this case is nothing but

the well-known Mukhanov-Sasaki variable: Its usual definition $v_{\boldsymbol{k}} = \sqrt{1+w}a^{-\frac{1}{2}(1-3w)}\phi_{\boldsymbol{k}}$ indeed becomes

$$v_{\boldsymbol{k}} = -\sqrt{\frac{3(w+1)}{w\kappa_0}}a\mathcal{R}_{\boldsymbol{k}}, \tag{24}$$

so that the function v/a, whose spectrum we compute below, can be identified, up to an irrelevant constant, with the curvature perturbation on the comoving hypersurfaces.

One can introduce the quantization of the background following a two step procedure: One first replaces the zeroth order quantities by the corresponding operators using the rules

$$\begin{aligned} q^\alpha &\mapsto \hat{Q}^\alpha, \\ q^\alpha p^2 &\mapsto \left[\hat{Q}^\alpha \hat{P}^2 - i\hbar\alpha\hat{Q}^{\alpha-1}\hat{P}\right] + \mathfrak{c}(\alpha)\hat{Q}^{\alpha-2}, \end{aligned} \tag{25}$$

in which $\mathfrak{c}(\alpha) \propto \hbar^2$ is positive. One way to determine $\mathfrak{c}(\alpha)$ is from the canonical quantization rules that impose symmetrization of the operator with respect to $\hat{Q}$ and $\hat{P}$. However, as in the case of the Hamiltonian (8), canonical prescription is not well-justified in this case either: The (q, p)-phase space admits affine symmetry rather than the Weyl-Heisenberg symmetry. Affine quantization based on the operators $\hat{Q}$ and $\hat{D}$ is a more suitable approach, respecting the covariance of the system with respect to the affine transformations. This method results in largely arbitrary $\mathfrak{c}(\alpha)$, introducing a quantization ambiguity. Details of this procedure are to be found in a dedicated Appendix of Ref. [1]. We can conveniently constrain this parameter; however, its unrestricted choice does not seem to impact the qualitative behavior of the system. From now on, we move to natural units in which $\hbar = 1$.

Combining this step with the usual quantization of the perturbation variables $v_{\boldsymbol{k}}$ and $\pi_{v,\boldsymbol{k}}$ maps the classical Hamiltonian (21) into a quantum one:

$$\hat{H}^{(2)}_{\boldsymbol{k}} = \frac{1+w}{2}\left(\frac{\hat{Q}}{\gamma}\right)^{2r}\left(|\hat{\pi}_{v,\boldsymbol{k}}|^2 + \hat{\Omega}_r^2|\hat{v}_{\boldsymbol{k}}|^2\right), \tag{26}$$

with

$$\begin{aligned} \hat{\Omega}_r^2 = &\left(\frac{\hat{Q}}{\gamma}\right)^{4(r_{\rm F}-r)} wk^2 + \frac{r(r+1)(4\kappa_0)^2}{(1+w)^2}\left(\frac{\hat{Q}}{\gamma}\right)^{-4r} \\ &\times \hat{Q}^{-2}\left[\hat{P}^2 + 2i(r+1)\hat{Q}^{-1}\hat{P} + \mathfrak{c}(-2r-2)\hat{Q}^{-2}\right], \end{aligned} \tag{27}$$

where the parameter $\mathfrak{c}(-2r-2)$, calculable from affine quantization, is unknown at this stage.

The second step consists in averaging the corresponding operator (function of $\hat{Q}$ and $\hat{P}$) in the semiquantum state $|q(\tau), p(\tau)\rangle$, leading to a Hamiltonian depending only on the perturbation variables, the background being then described by a trajectory. In practice, we use the definition

$$H^r_{\boldsymbol{k}}(\tau) \coloneqq \langle q(\tau), p(\tau)|\hat{H}^{(2)}_{\boldsymbol{k}}|q(\tau), p(\tau)\rangle, \tag{28}$$

and assume the parametric phase-space trajectory $\{q(\tau), p(\tau)\}$ to be given by the solutions (11).

Applying to these classically equivalent formulations the two-step quantization procedure discussed above, and upon canonical quantization of the variable $v_{\boldsymbol{k}}$, one finds

$$H^r_{\boldsymbol{k}}(\tau) = \frac{1+w}{2}\left(\frac{q}{\gamma}\right)^{2r}\left(\mathfrak{M}_r|\hat{\pi}_{v,\boldsymbol{k}}|^2 + \breve{\Omega}_r^2|\hat{v}_{\boldsymbol{k}}|^2\right), \tag{29}$$

where

$$\begin{aligned} \breve{\Omega}_r^2 = &\mathfrak{L}_r\left(\frac{q}{\gamma}\right)^{4(r_{\rm F}-r)} wk^2 + \frac{r(r+1)(4\kappa_0)^2}{q^2(1+w)^2}\left(\frac{q}{\gamma}\right)^{-4r} \\ &\times\left(\mathfrak{N}_r p^2 + \frac{\mathfrak{T}_r}{q^2}\right), \end{aligned} \tag{30}$$

and $\mathfrak{L}_r$, $\mathfrak{M}_r$, $\mathfrak{N}_r$, $\mathfrak{T}_r$ are four arbitrary semiclassical parameters that encode ambiguities in both the quantization process (27) and the semiclassical transition through unspecified coherent states (9) (see again Ref. [1] for details).

Expanding $\hat{v}_k$ in creation and annihilation operators yields the evolution for the mode functions, denoted $v_k(\tau)$, which only depend on the amplitude $k = |\boldsymbol{k}|$ of the wave vector and not the direction $\boldsymbol{k}/k$. All the above models can be easily compared provided one rescales the respective mode functions $v_k(\tau)$ to a common variable, the Mukhanov-Sasaki variable introduced above and denoted by $\tilde{v}_k(\tau)$. The mode functions $v_k(\tau)$ satisfy the semiclassical equations of motion stemming from the Hamiltonian (29). It can be rescaled via the transformation

$$\tilde{v}_k = \left(\frac{q}{\gamma}\right)^{r_{\rm F}-r} v_k, \tag{31}$$

thereby defining $\tilde{v}_k$. Then, using the conformal time defined through Eq. (23) above, one finds that the mode equation for $\tilde{v}_k$ becomes

$$\tilde{v}_k'' + (\mathfrak{M}_r\mathfrak{L}_r wk^2 - \mathcal{V})\tilde{v}_k = 0,$$

with the potential reading

$$\mathcal{V} = -\frac{(4\kappa_0)^2}{(1+w)^2q^2}\left(\frac{q}{\gamma}\right)^{-4r_{\rm F}}\left(\mathcal{A}_r p^2 + \frac{\mathcal{B}_r}{q^2}\right), \tag{32}$$

with

$$\mathcal{A}_r = (r_{\rm F}-r)(1+r_{\rm F}+r) + \mathfrak{M}_r\mathfrak{N}_r r(r+1),$$

and

$$\mathcal{B}_r = \mathfrak{T}_r\mathfrak{M}_r r(r+1) - (r_{\rm F}-r)\mathfrak{K}.$$

The classical limit (21) can be recovered for $q \to \infty$ by sending $\mathcal{A}_r$ to unity, which in turn, can be achieved by rescaling the conformal time through $\eta \to \eta/\sqrt{\mathcal{A}_r}$; this demands we assume $\mathcal{A}_r > 0$. Similarly, one can absorb the irrelevant constant into a redefinition of the wave number $k\sqrt{w\mathfrak{L}_r\mathfrak{M}_r\mathcal{A}_r^{-1}} \to k$. This leads to a Mukhanov-Sasaki mode equation

$$\tilde{v}_k'' + (k^2 - \mathcal{V}_\chi)\tilde{v}_k = 0, \tag{33}$$

with a potential $\mathcal{V}_\chi$ given by

$$\mathcal{V}_\chi = -\frac{(4\kappa_0)^2}{(1+w)^2 q^2}\left(\frac{q}{\gamma}\right)^{-4r_\mathrm{F}}\left(p^2 + \frac{\chi\mathfrak{K}}{q^2}\right), \tag{34}$$

depending on the chosen value of the otherwise arbitrary number r; explicitly, it reads

$$\chi = \frac{\mathfrak{K}^{-1}\mathcal{B}_r}{\mathcal{A}_r} = \frac{\mathfrak{T}_r\mathfrak{M}_r\mathfrak{K}^{-1}r(r+1) - (r_\mathrm{F} - r)}{\mathfrak{M}_r\mathfrak{N}_r r(r+1) + (r_\mathrm{F} - r)(r_\mathrm{F} + r + 1)}. \tag{35}$$

We are thus left with a single parameter χ reflecting the quantization ambiguity induced by the free choice of basic perturbation variables to be quantized, which depends on r. We note that χ can be both positive and negative, both cases being consistent with affine symmetry and admitting the classical limit. Neither appears to be preferred.

Upon using the background solution (11) and expressing $\mathfrak{K}$ and H_sem in terms of q_B, ω, and κ_0, namely

$$\mathfrak{K} = \frac{q_\mathrm{B}^4\omega^2}{16\kappa_0^2} \quad \text{and} \quad H_\mathrm{sem} = \frac{q_\mathrm{B}^2\omega^2}{8\kappa_0},$$

Eq. (34) becomes

$$\mathcal{V}_\chi = \frac{2\omega^2}{9Z_{r_\mathrm{F}}^4}\frac{1-3w}{(1-w)^2}\frac{\chi + (\omega\tau)^2}{[1+(\omega\tau)^2]^2}, \tag{36}$$

with Z_{r_F} given by (20).

One can also note that the potential $\mathcal{V}_\chi$ in (36) can be given a simple form for an arbitrary χ, namely

$$\mathcal{V}_\chi = \frac{2(1-3w)\chi^2}{9(1-w)^2[1+(1+2r_\mathrm{F})\chi]}\frac{\left(q^{\frac{1}{\chi}+r_\mathrm{F}+r_\mathrm{C}}\right)''}{q^{\frac{1}{\chi}+r_\mathrm{F}+r_\mathrm{C}}}, \tag{37}$$

with

$$r_\mathrm{C} = 1 + r_\mathrm{F} = \frac{2}{3(1-w)}, \tag{38}$$

implying $\frac{2}{3} \le r_\mathrm{C} \le 1$ with $0 \le w \le \frac{1}{3}$. One can easily check that for $w \in]-\frac{1}{3}, \frac{1}{3}[$, the prefactor is positive definite.

As discussed in Ref. [1], there are two special values for χ, namely $\chi_\mathrm{F} = -1/r_\mathrm{C} = -\frac{3}{2}(1-w) < 0$, the value obtained for $r = 0$, for which the potential, we denote by $\mathcal{V}_\mathrm{F}$, turns out to be $\mathcal{V}_\mathrm{F} = (q^{r_\mathrm{F}})''/q^{r_\mathrm{F}}$, and $\chi_\mathrm{C} = -1/r_\mathrm{F} = 3(1-w)/(1-3w) > 0$, corresponding to the choice $r = r_\mathrm{F}$, leading to $\mathcal{V}_\mathrm{C} = (q^{r_\mathrm{C}})''/q^{r_\mathrm{C}}$. The prefactor is unity at these points, with a vanishing minimum at $\chi = 0$. A few cases are displayed in Fig. 1.

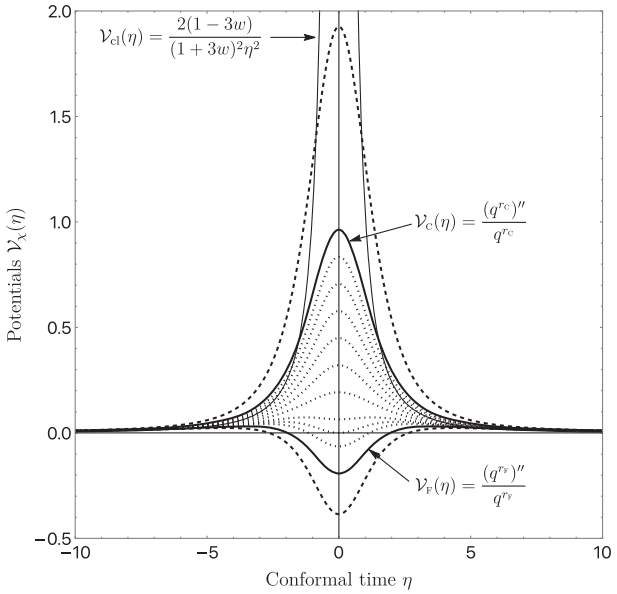

FIG. 1. The potential $\mathcal{V}_\chi$ sourcing the perturbations for $w = 0.2$ and different values of the phenomenological parameter χ. They all converge far from the bounce where they behave as $\mathcal{V}_\mathrm{cl}$ [Eq. (39)] shown as a thin line. The two extreme with $\chi = \chi_\mathrm{F}(w)$ and $\chi = \chi_\mathrm{C}(w)$ are shown as full thick lines, while the dotted curves represent a selection of values between these extreme. The dashed curves are for $\chi < \chi_\mathrm{F}$ and $\chi > \chi_\mathrm{C}$.

The specific form of the potentials with unit prefactor enables an analytical approach to perturbation dynamics while representing two distinct dynamical situations; this is expanded upon in Sec. III B. These values naturally reproduce the degenerate classical case $q \to q_\mathrm{cl}$ (i.e., for large $|\eta|$), namely

$$\mathcal{V}_\mathrm{cl} = \frac{(q_\mathrm{cl}^{r_\mathrm{F}})''}{q_\mathrm{cl}^{r_\mathrm{F}}} = \frac{(q_\mathrm{cl}^{r_\mathrm{C}})''}{q_\mathrm{cl}^{r_\mathrm{C}}} = \frac{2(1-3w)}{(1+3w)^2\eta^2}, \tag{39}$$

with q_cl and p_cl the classical solutions (7). We shall however in what follows assume that χ is an arbitrary real parameter and restrict attention to these particular cases whenever necessary. Figure 1 emphasizes some possible cases with $\chi_\mathrm{F} < \chi < \chi_\mathrm{C}$, together with two examples for $\chi < \chi_\mathrm{F}$ and $\chi > \chi_\mathrm{C}$, illustrating that the points χ_C and χ_F do not lead to anything particular apart from the fact that they permit a simple writing of the potential. In fact, in the large time limit $\omega\tau \gg 1$, the term proportional to χ in both Eqs. (34) and (36) is in any way negligible, and it can be checked explicitly that the classical case (39) is also recovered for any value of χ.

The ambiguity is clear from Fig. 1: The parameter χ stems from the arbitrary choice that is made among various classically equivalent theories to quantize. Once this choice is made, and the factor ordering is taken care of, the potential for the perturbations is completely fixed, but it depends on the actual value of χ, which is *a priori* not fixed by any physical principle. The resulting spectrum, to which we now turn, therefore also depends on this unphysical parameter, thereby leading to ambiguous physical predictions.

A more detailed examination of Eq. (35) however shows that the ambiguity is twofold. Using the so-called "fluid parametrization" $r = 0$ yields $\chi = \chi_{\rm F} < 0$, which is entirely fixed once the barotropic index of the equation of state w and the background solution (11) are known. On the other hand, the conformal case $r = r_{\rm F}$ depends on $\chi = \mathfrak{T}_{r_{\rm F}}/(\mathfrak{K}\mathfrak{N}_{r_{\rm F}})$, which is not fixed by the background but rather by the quantization procedure. The special case $\chi \to \chi_{\rm C} = \frac{3(1-w)}{1-3w} > 0$, again solely fixed by the equation of state, belongs to the second category and will be called in what follows "conformal parametrization."

C. Discussion

Let us conclude the present section by emphasizing the quantum origin of our new ambiguity.

First, we introduced a set of different basic variables for the perturbation field through Eq. (17). They all represent equally valid choices, their dynamics being, as expected, generated by different Hamiltonians (18) that involve different background observables for coupling the perturbation variables to the background spacetime. Next, we quantized the background observables with the quantization prescription (25), in which ordering ambiguities are taken care of by fixing the parameter of Eq. (25). On comparing the mode functions associated with different basic field variables, we found that their dynamical equations given in Eq. (33) are inequivalent because of the ambiguous gravitational potential (34). Had the background observables been classical, there would have been no dynamical ambiguity. Indeed, the dynamics of the mode functions in classical backgrounds is unique, and the redefinition of the basic field variables merely transforms the vacuum state of the perturbation field, as discussed, e.g., in Ref. [6]. We conclude that it is the quantum spacetime that is responsible for the dynamical ambiguity whose physical consequence we study in the following sections.

In more explicit details, as shown both diagrammatically through Fig. 2 and analytically in the Appendix, the theory described by Eq. (13) is canonically transformed, classically speaking, into Eq. (18) and subsequently quantized to yield the semiclassical Hamiltonian (29). Instead, starting from the quantum version of Eq. (13) upon substituting $q \to \hat{Q}$ and $p \to \hat{P}$ at the background level,

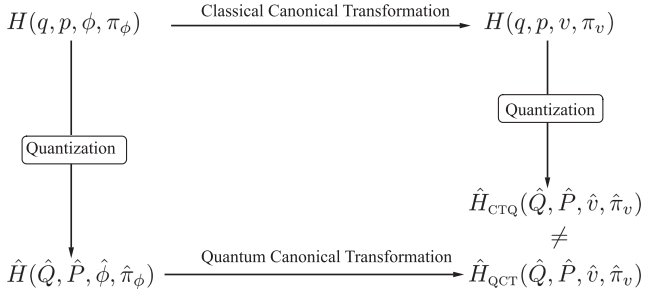

FIG. 2. The origin of our ambiguity explained by the process through which one changes variables: Starting with a given classical first order theory with Hamiltonian $H(q,p,\phi,\pi_\phi)$ depending on background (q,p) and perturbation (ϕ,π_ϕ) variables, one can either perform a classical canonical transformation and quantize the resulting theory or first quantize the original theory and subsequently perform a quantum canonical transformation. These operations in general lead to different quantum theories.

but also $\phi_{\boldsymbol{k}} \to \hat{\phi}_{\boldsymbol{k}}$ and $\pi_{\phi,\boldsymbol{k}} \to \hat{\pi}_{\phi,\boldsymbol{k}}$ for the perturbations, the quantum canonical unitary transformation [3]

$$U_{\boldsymbol{k}} = \exp\left(i\alpha\hat{D}_{v,\boldsymbol{k}}\right)\exp\left(i\beta\hat{v}_{\boldsymbol{k}}^2\right), \tag{40}$$

with $\alpha = \alpha(\hat{Q},\hat{P})$ and $\beta = \beta(\hat{Q},\hat{P})$ Hermitian operators ($\alpha^\dagger = \alpha$, $\beta^\dagger = \beta$) depending only on the background variables and

$$\hat{D}_{v,\boldsymbol{k}} := \frac{1}{2}\left(\hat{v}_{\boldsymbol{k}}\hat{\pi}_{v,\boldsymbol{k}} + \hat{\pi}_{v,\boldsymbol{k}}\hat{v}_{\boldsymbol{k}}\right) \tag{41}$$

yields, to second order in perturbations, the quantum Hamiltonian (A15). The Appendix includes some details on the application of the above transformation to the quantized Hamiltonian (13). The perturbation variables, to first order, transform as

$$\begin{aligned}\hat{\phi}_{\boldsymbol{k}} &= U^\dagger\hat{v}_{\boldsymbol{k}}U = \mathrm{e}^{-\alpha}\hat{v}_{\boldsymbol{k}} + \cdots,\\ \hat{\pi}_{\phi,\boldsymbol{k}} &= U^\dagger\hat{\pi}_{v,\boldsymbol{k}}U = \mathrm{e}^{\alpha}\hat{\pi}_{v,\boldsymbol{k}} + (\beta\mathrm{e}^{\alpha} + \mathrm{e}^{\alpha}\beta)\hat{v}_{\boldsymbol{k}} + \cdots.\end{aligned} \tag{42}$$

Setting $\alpha = \ln[\sqrt{1+w}(\hat{Q}/\gamma)^r]$ and $\beta = -\frac{1}{4}\partial_\tau[\exp(-2\alpha)]$ shows that, in the classical limit, the relations (42) indeed become identical with the relations (17) [where Z is given by Eq. (20)]. If the only quantized variables were the perturbation variables for which both the classical and the quantum canonical transformations are linear, then the quantum motion generated by the respective quadratic Hamiltonians would be unique irrespective of whether the choice of perturbation variables is made at the classical or quantum level (as shown in Ref. [6]). This is so because there exists a homomorphism between the Poisson algebra of polynomial phase space observables of degree no greater than 2 and the brackets of corresponding operators (see, e.g., [7] for more details). On the other hand, it is known

that if a quantum unitary transformation is nonlinear or/and the Hamiltonian is not quadratic, then the homomorphism breaks down, which results in the noncommutativity depicted in Fig. 2. In such cases, the quantum motion depends on whether the choice of basic variables is made at the classical or quantum level. If we view the quantum canonical transformation (42), or the Hamiltonian (A1), from the perspective of the full Hilbert space $\mathcal{H}_{\rm B}\otimes\mathcal{H}_{\rm P}$, mixing background and perturbation degrees of freedom, we note that they are higher order in basic variables as they involve quantum background and perturbation variables. Hence, we ascribe the source of the ambiguity to the long known quantization obstructions (the so-called Groenewold-Van Hove obstructions [26,27]).[2]

III. GETTING SPECTRAL INDICES

After having summarized the situation, let us now solve the quantum dynamics of the perturbation modes, which we do first numerically and then analytically. We investigate the amplitude of the perturbations as a function of time for various wave numbers k and focus on its dependency on the free parameter of the conformal parametrization χ.

We shall work in the Heisenberg picture of dynamics and assume the perturbations to be in a fixed vacuum state that is the ground state of the quantum Hamiltonian (13) or (29) for all modes of interest in the large contracting Universe ($\eta\to-\infty$). It can be shown that in order for the vacuum state to be the ground state of the quantum Hamiltonians in the infinite past $\tau,\eta\to-\infty$, the mode functions have to satisfy (up to irrelevant phase), respectively,

$$v_k^\chi|_{\eta_{\rm ini}}=\frac{1}{\sqrt{2k}}\quad\text{and}\quad\left.\frac{{\rm d}v_k^\chi}{{\rm d}\eta}\right|_{\eta_{\rm ini}}=i\sqrt{\frac{k}{2}},\tag{43}$$

where we used the vanishing of the gravitational potential in the infinite past.[3] Equipped with the initial conditions (43), we now proceed to solve the mode equation (33) for the two special cases $\chi\to\chi_{\rm F}$ and $\chi\to\chi_{\rm C}$.

A. Numerical integration

Since the potential $\mathcal{V}_\chi$ is known explicitly as a function of the internal time τ as shown in Eq. (36), it turns out to be technically more tractable to switch back to τ to solve Eq. (33), even though, for the sake of clarity, we plot the results in terms of the conformal time, substituting the numerical value for $\tau(\eta)$ in the solution. Given the relationship (23) between both times, we have ${\rm d}/{\rm d}\eta=Z^{-2}{\rm d}/{\rm d}\tau$ (we assume, from now on, that $Z=Z_{r_{\rm F}}$) and therefore,

$$\frac{{\rm d}^2}{{\rm d}\eta^2}=\frac{1}{Z^4}\frac{{\rm d}^2}{{\rm d}\tau^2}-\frac{1}{Z^6}\frac{{\rm d}Z^2}{{\rm d}\tau}\frac{\rm d}{{\rm d}\tau},\tag{44}$$

so that the perturbation equation of motion for the Mukhanov-Sasaki variable, namely

$$\frac{{\rm d}^2v_k^\chi}{{\rm d}\eta^2}+[k^2-\mathcal{V}_\chi(\eta)]v_k^\chi=0,\tag{45}$$

reads, plugging the semiquantum solution (11) for the generic χ-parametrization (with $\chi={\rm F}$ or C),

$$\frac{{\rm d}^2v_k^\chi}{{\rm d}x^2}-\frac{2r_{\rm F}x}{1+x^2}\frac{{\rm d}v_k^\chi}{{\rm d}x}+\left[\left(\frac{q_{\rm B}}{\gamma}\sqrt{1+x^2}\right)^{4r_{\rm F}}(1+w)^2\tilde{k}^2-\frac{2\omega^2(1-3w)}{9(1-w)^2}\frac{\chi+x^2}{(1+x^2)^2}\right]v_k^\chi=0,\tag{46}$$

where we set $\tilde{k}:=k/\omega$ as well as $x:=\omega\tau$. In what follows, we drop the index χ on the mode as there is no risk of confusion; we will merely specify when we explicitly calculate for the fluid or conformal parametrization.

Once the initial conditions (43) are similarly expressed in terms of the fluid time τ, the numerical integration of the above equations allows to follow the dynamics of the stochastic average

$$\langle\mathcal{R}_{\boldsymbol{k}}\mathcal{R}^*_{\boldsymbol{k}'}\rangle=\mathcal{P}_{\mathcal{R}}(k)\delta_{\boldsymbol{k},\boldsymbol{k}'},\tag{47}$$

providing the amplitude of curvature perturbations (we follow the convention of Ref. [28], up to an irrelevant normalization factor)

$$\delta_\chi[k,\tau(\eta)]=\sqrt{\mathcal{P}_{\mathcal{R}}(k)}=\frac{|v_k|}{a}k^{3/2}=k^{3/2}|v_k|\left(\frac{q}{\gamma}\right)^{-r_{\rm C}},\tag{48}$$

where we made use of the definition (4) of the scale factor a in terms of the variable q. We focus in this section to the special cases $\chi=\chi_{\rm F}$ and $\chi=\chi_{\rm C}$.

Although the amplitude is dynamical, it reaches a plateau right after the bounce when the perturbations have been amplified and thus remains roughly constant for a

[2] In Ref. [7], the quantized phase space is $\mathbb{R}^{2n}$, whereas in our case, it is $(q,p,\phi_{\boldsymbol{k}},\pi_{\phi,\boldsymbol{k}})\in\mathbb{R}_+\times\mathbb{R}^3$. We, however, use the dilation operator $\hat{D}$ as a basic quantum variable that combined with $\ln\hat{Q}$ satisfies the canonical commutation rule and brings our case to that of [7].

[3] The initial conditions of Eq. (43), are, strictly speaking, approximate in the general situation. In the fluid parameterization, for instance, the time derivative should read

$$\frac{{\rm d}v_k^{\rm F}}{{\rm d}\eta}=i\sqrt{\frac{k}{2}}-\frac{1}{(1+w)\sqrt{2k}}\frac{1}{q^{-r_{\rm F}}}\frac{\rm d}{{\rm d}\eta}(q^{-r_{\rm F}}),$$

the second term originating from the fact that it is the field ϕ rather than v that is quantized in this case. As initial conditions are set for $|\tau|\gg1$, one can thereby use the asymptotic behaviors $\dot{q}/q\sim\tau^{-1}$ and $\eta\sim\tau^{r_{\rm F}+r_{\rm C}}$, (see Ref. [1]) to write the extra term in the time derivative of $v_k^{\rm F}$ as $(3w-1)/[(1+w)(1+3w)\sqrt{k}\eta]$: Setting initial conditions sufficiently deep into the contracting phase ($\eta<0$ and $|\eta|\gg1$) then permits to neglect such a term for all parameterizations.

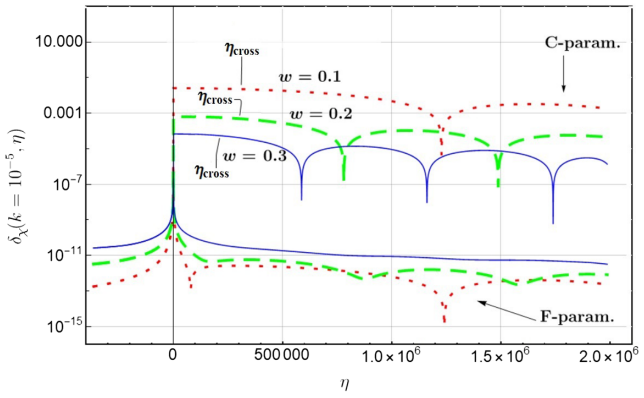

FIG. 3. Conformal time development of the perturbation amplitude (48) for the mode $k = 10^{-5}$ and three different equation of state parameters, namely $w = 0.1$ (dotted), $w = 0.2$ (dashed), and $w = 0.3$ (solid). Both parametrizations, fluid (bottom, $\chi = \chi_{\rm F}$) and conformal (top, $\chi = \chi_{\rm C}$), are shown. Also indicated is the time $\eta_{\rm cross}$ at which the mode exits the potential, i.e., for which $\mathcal{V}(\eta_{\rm cross}) = k^2$. Here and in the following figures, the background parameters used are fixed by setting $\kappa_0 \to 1$, $H_{\rm sem} = 2^{1+w}$ and $\mathfrak{K} = 100$ in (11).

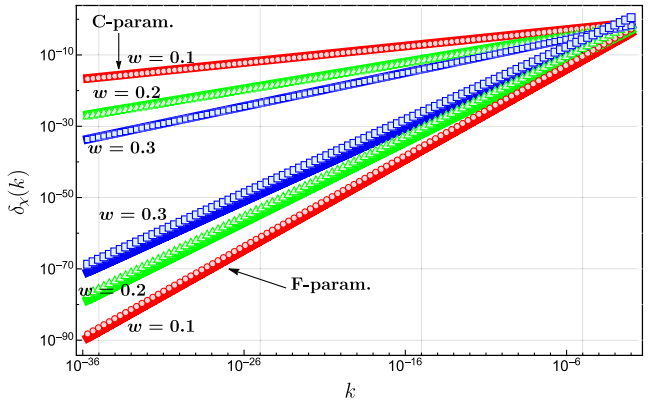

FIG. 4. Primordial density fluctuation power spectrum $\delta[k, \tau(\eta_{\rm cross})]$ measured at the crossing time $\eta_{\rm cross}$ defined in Eq. (51) and shown in Fig. 3. Both the fluid F-(bottom) and the conformal C-(top) parametrizations are displayed for three different fluids as in Fig. 3, namely $w = 0.1$ (circles), $w = 0.2$ (triangles), and $w = 0.3$ (squares). The approximate analytical solutions [Eqs. (69) and (68) below] are shown as superimposed solid lines for each numerical calculation, exemplifying the validity of the approximation.

significant fraction of its period; this corresponds to the constant (or growing) mode when the perturbation is dominated by the potential. This is illustrated in Fig. 3, where the dynamics of the amplitude of a selected mode in both parametrizations and for three different equation of state parameter w. This constant value of the amplitude right after the bounce is called the primordial amplitude, and we shall study its dependence on the wave number k.

We have solved the perturbation equations for many values of k and calculated their primordial amplitude at the time of potential crossing (also called "exit" time) $\eta_{\rm C}$ at which the mode exits the potential, i.e., for which $\mathcal{V}(\eta_{\rm C}) = k^2$. The mode evolutions shown in Fig. 3 yield the full spectrum, plotted in Fig. 4. One finds two different power laws for the two different parametrizations, as expected, thereby emphasizing the ambiguity at the prediction level. Our analytic estimates below for the spectral indices represent very accurate fits for the numerics.

B. Analytical integration

We now follow the calculation made in Ref. [2] for the case of tensor perturbations, transcribed to the scalar modes, consisting in setting a piecewise approximation to the solution of our general differential equation

$$\frac{{\rm d}^2 v_k}{{\rm d}\eta^2} + \left[k^2 - \frac{(q^r)''}{q^r}\right] v_k = 0, \tag{49}$$

where we set the prefactor in the potential is sent to unity as we are only interested in the solution for $r = r_{\rm F}$ and $r = r_{\rm C}$; see discussion below Eq. (38). We begin by noticing that long before the bounce, at times for which the modes are free, i.e., when $k^2 \gg |\mathcal{V}|$, the potential is well approximated by its classical counterpart (39). In this regime, the modes are then given by

$$v_k(\eta) = \sqrt{-\eta}\left[c_1 H_\nu^{(1)}(-k\eta) + c_2 H_\nu^{(2)}(-k\eta)\right], \tag{50}$$

where $\nu = \frac{3(1-w)}{2(1+3w)}$ and $H_\nu^{(1,2)}$ are the Hankel functions of the first and second kinds; the minus signs appearing in Eq. (50) account for the fact that $\eta < 0$ in the contracting phase. Since, for $(-k\eta) \gg 1$, one has the asymptotic relations $H_\nu^{(1)}(-k\eta) \sim \sqrt{\frac{-2}{k\eta\pi}} {\rm e}^{-i[k\eta+(\nu+\frac{1}{2})]}$ and $H_\nu^{(2)}(-k\eta) \sim \sqrt{\frac{-2}{k\eta\pi}} {\rm e}^{i[k\eta+(\nu+\frac{1}{2})]}$, the initial conditions (43) that impose the Bunch-Davies vacuum yield $c_1 = 0$ and $c_2 = \sqrt{\pi/2}\, e^{-i\frac{\pi}{2}(\nu+\frac{1}{2})}$. This implies that at the time $\eta_{\rm in} = -\eta_{\rm cross}$ of the potential crossing $k^2 = \mathcal{V}(\eta_{\rm cross})$, namely

$$\eta_{\rm cross} = \frac{\sqrt{2(1-3w)}}{(1+3w)k} =: \frac{x_w}{k}, \tag{51}$$

thereby defining the dimensionless variable x_w depending only on the equation of state w, the initial conditions for the following potential domination era read

$$v_k(\eta_{\rm in}) = \frac{C}{\sqrt{k}} \quad \text{and} \quad v_k'(\eta_{\rm in}) = D\sqrt{k}, \tag{52}$$

where

$$C = c_2 \sqrt{x_w} H_\nu^{(2)}(x_w), \tag{53}$$

and

$$D = \frac{c_2}{2}\left\{\frac{H_\nu^{(2)}(x_w)}{\sqrt{x_w}} + \sqrt{x_w}\left[H_{\nu-1}^{(2)}(x_w) - H_{\nu+1}^{(2)}(x_w)\right]\right\}. \quad (54)$$

From the potential crossing conformal time $\eta_{\rm cross}$, one can derive the fluid time $\tau_{\rm cross}$, which depends on the wave number k of a given mode. In the classical approximation, i.e., assuming this crossing takes place in a regime for which the potential is well approximated by the classical potential (39), one finds

$$x_{\rm cross} = \omega\tau_{\rm cross} = \left(\frac{q_{\rm B}}{\gamma}\right)^{\frac{2(1-3w)}{1+3w}}\left[\frac{k}{\omega f(w)}\right]^{-\frac{3(1-w)}{1+3w}}, \quad (55)$$

where $f(w) = \sqrt{2(1-3w)}/[3(1-w^2)]$.

Once a given mode crosses the potential, we assume the latter to instantaneously take over the dynamics of the perturbations, so that Eq. (49) becomes (zeroth-order in k):

$$\frac{{\rm d}^2 v_k}{{\rm d}\eta^2} - \frac{(q^r)''}{q^r} v_k = 0, \quad (56)$$

whose general solution is found to be

$$v_k = [q(\eta)]^r\left\{A + B\int^\eta {\rm d}\tilde{\eta}[q(\tilde{\eta})]^{-2r}\right\}, \quad (57)$$

where A and B are integration constants, later to depend on k because of the matching with initial conditions.

In order to use the solution (57), one needs to express the background motion of q given by Eq. (11) as a function of the conformal time η. It turns out that Eq. (23) can be integrated to yield

$$\eta = (1+w)\left(\frac{q_{\rm B}}{\gamma}\right)^{2r_{\rm F}}\tau\mathcal{F}\left[\frac{1}{2}, -r_{\rm F}; \frac{3}{2}; -(\omega\tau)^2\right],$$

with $\mathcal{F}$ an hypergeometric function (see Ref. [1] for details). We can perform the integrals in fluid time using the relation (23) and obtain the solutions in terms of τ, absorbing the choice of the initial time η_0 into the constants

$$v_k = \left(\frac{q}{\gamma}\right)^r\left\{A_k + \omega\tau\mathcal{F}\left[\frac{1}{2}, r-r_{\rm F}; \frac{3}{2}; -(\omega\tau)^2\right]B_k\right\}, \quad (58)$$

where

$$A_k = A \quad \text{and} \quad B_k = \frac{B}{\omega(1+w)}\left(\frac{q_{\rm B}}{\gamma}\right)^{2(r-r_{\rm F})}$$

are unknown functions of the wave number k.

The solution (58) is valid for both the above parametrizations, and setting $r \to r_{\rm F}$ (fluid) or $r \to r_{\rm C} = 1 + r_{\rm F}$ (conformal) yields

$$v_k^{\rm F} = \left(\frac{q}{\gamma}\right)^{r_{\rm F}}\left(A_k^{\rm F} + B_k^{\rm F}\tau\right) \quad (59)$$

and

$$v_k^{\rm C} = \left(\frac{q}{\gamma}\right)^{r_{\rm C}}\left[A_k^{\rm C} + B_k^{\rm C}\,\arctan(\omega\tau)\right]. \quad (60)$$

Given the form (48) of the amplitude of curvature perturbations, one needs to evaluate $(q/\gamma)^{-r_{\rm C}}|v_k|$ in the large time limit, which yields

$$\delta_\chi \propto \left[A_k \pm \frac{\sqrt{\pi}}{2}\frac{\Gamma\left(r-r_{\rm F}-\frac{1}{2}\right)}{\Gamma(r-r_{\rm F})}B_k\right]|\omega\tau|^{r-r_{\rm C}} + B_k\frac{{\rm e}^{-2i\pi(r-r_{\rm F})}}{1-2(r-r_{\rm F})}|\omega\tau|^{r_{\rm F}-r}, \quad (61)$$

in which the $\pm$ sign in the first line corresponds to the sign of τ. One notes that for the values of interest $r = r_{\rm F}$ and $r = r_{\rm C}$, this amplitude reads (recall $r_{\rm C} - r_{\rm F} = 1$)

$$\delta_{\rm F} = \delta_{\chi_{\rm F}} \propto \frac{A_k^{\rm F}}{|\omega\tau|} + B_k^{\rm F} \quad (62)$$

and

$$\delta_{\rm C} = \delta_{\chi_{\rm C}} \propto \left(A_k^{\rm C} \pm \frac{\pi}{2}B_k^{\rm C}\right) - \frac{B_k^{\rm C}}{|\omega\tau|}. \quad (63)$$

These two distinct solutions both exhibit a constant mode and a decaying one and therefore provide a constant amplitude for the primordial spectrum.

As we assume $w < 1/3$, the potential (36) is positive definite for $\chi > 0$ with a maximum at $\eta = 0$. For $\chi < 0$, on the other hand, this potential has two positive maxima and a negative minimum at $\eta = 0$ so that the modes cross the potential at four different times (see Fig. 1). Given the symmetry of $V_\chi(\eta)$, the relevant modes enter the potential for the first time at $\eta_{\rm in} = -\eta_{\rm C}$ and exit for the last time at $\eta_{\rm out} = \eta_{\rm C}$ in regions where it behaves classically (i.e., for $|\omega\tau| \ll 1$). Figure 1 also shows that for a range of values of r, including in particular the fluid parametrization, the modes also exit and reenter the potential another time between those points, when quantum corrections cannot be neglected. Due to the shape of the potential, there exist short periods of time during which the value of k dominates over the value of $V_\chi(\eta)$, i.e., in the neighborhoods of $\pm\eta_0$ defined by $V_\chi(\pm\eta_0) = 0$. It turns out the potential is rather steep close to those points, with a high negative slope when the modes exit and a high positive slope when they reenter later. For the large wavelengths relevant to the cosmological framework, this time interval is sufficiently small that the approximation, assumed in what follows, of neglecting it altogether, holds. It should be mentioned, however, that in

that case, the potential becoming negative, the behaviors of the modes may be quite different; we shall see below how this should be taken care of.

Combining the matching conditions (52) at the time (55) with the potential-domination solutions (59) and (60) yields the coefficients A^{F}, A^{C}, B^{F}, and B^{C} as functions of k. To leading order in $k \ll 1$, one gets

$$A_k^{\mathrm{F}} = \left(\frac{q_{\mathrm{B}}\omega f}{\gamma}\right)^{\frac{1-3w}{1+3w}} \left[r_{\mathrm{C}} C + (1+w) f D\right] k^{-\frac{3(1-w)}{2(1+3w)}} \tag{64}$$

and

$$B_k^{\mathrm{F}} = f \left(\frac{q_{\mathrm{B}}\omega f}{\gamma}\right)^{-\frac{1-3w}{1+3w}} \left[r_{\mathrm{F}} C + (1+w) f D\right] k^{\frac{3(1-w)}{2(1+3w)}}. \tag{65}$$

We note that A_k^{F} and B_k^{F} have inverse k dependence so that, in the large wavelength limit, $A_k^{\mathrm{F}} \gg B_k^{\mathrm{F}}$. For the conformal case, one finds

$$A_k^{\mathrm{C}} = \frac{\pi}{2} B_k^{\mathrm{C}} + C \left(\frac{q_{\mathrm{B}}}{\gamma}\right)^{-\frac{2}{1+3w}} k^{\frac{3(1-w)}{2(1+3w)}} \tag{66}$$

and $B_k^{\mathrm{C}} = \gamma A_k^{\mathrm{F}}/q_{\mathrm{B}}$, relations that can also be obtained by merely equating (59) and (60) and their derivatives at the matching point; we kept the subdominant term in B_k^{C} in (66) for further convenience.

The last step consists in substituting the above expressions into the primordial amplitude spectrum (48), keeping the highest order terms in $k \ll 1$, assuming $0 \leq w \leq \frac{1}{3}$. This yields

$$\delta_\chi(k) = A(w,\chi)\omega f \left(\frac{k}{\omega f}\right)^{n(w,\chi)}, \tag{67}$$

where the amplitudes

$$A(w,\chi_{\mathrm{F}}) = \left(\frac{q_{\mathrm{B}}}{\gamma}\right)^{-\frac{2}{1+3w}} |(r_{\mathrm{F}} + r_{\mathrm{C}}) C + 2(1+w) f D| \tag{68}$$

and

$$A(w,\chi_{\mathrm{C}}) = \pi \left(\frac{q_{\mathrm{B}}}{\gamma}\right)^{-\frac{6w}{1+3w}} |r_{\mathrm{C}} C + (1+w) f D|, \tag{69}$$

as well as the spectral indices

$$n(w,\chi_{\mathrm{F}}) = \frac{3(1+w)}{1+3w} \tag{70}$$

and

$$n(w,\chi_{\mathrm{C}}) = \frac{6w}{1+3w} \tag{71}$$

differ to yield effectively distinguishable predictions: The power spectrum being the square of the fractional energy density, i.e., $\mathcal{P}_{\mathrm{S}}(k) = \delta_\chi^2 \propto k^{n_{\mathrm{S}}-1}$, one finds two different power indices, namely that given by the fluid parametrization $n_{\mathrm{S}}^{\mathrm{F}} - 1 = 6(1+w_{\mathrm{F}})/(1+3w_{\mathrm{F}})$ (i.e., $w_{\mathrm{F}} \sim -0.988$ to agree with the CMB Planck data [29]), and $n_{\mathrm{S}}^{\mathrm{C}} - 1 = 12 w_{\mathrm{C}}/(1+3w_{\mathrm{C}})$ for the conformal one (i.e., $w_{\mathrm{C}} \sim -2.9 \times 10^{-3}$); it is the latter expression that is usually assumed [3]. Figure 4 shows, for various values of the equation of state parameter w, by superimposing the results, that the predicted spectra (68) and (69), agree with the numerical calculation.

IV. A TALE OF TWO INDICES

Solving Eq. (45) for arbitrary values of χ is not possible because of the prefactor in Eq. (37). As discussed there, there are two cases for which this prefactor is unity, namely for $\chi = \chi_{\mathrm{F}}$ and $\chi = \chi_{\mathrm{C}}$, and that the analytic solutions (57) are valid. Given that this parameter comes from the quantization process and is thus seemingly arbitrary, one may reasonably worry that the spectral index of scalar perturbations might depend on its exact value, the theory therefore loosing its predictive power. Indeed, for the two values for which one can solve the mode equation, one already obtains an ambiguity as the two spectral indices (70) and (71) are both possible predictions.

A. Numerical facts

Figure 5 shows the fluctuation δ_χ as a function of the wave number k for various values of χ. One immediately notices that although the amplitude depends on χ, decreasing with χ until χ_{F} and then increasing again for $\chi < \chi_{\mathrm{F}}$,

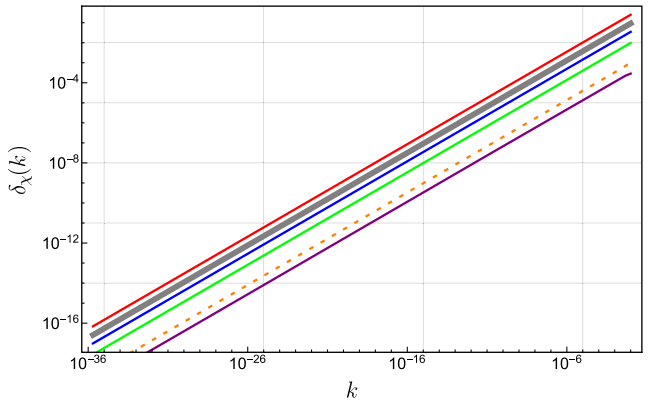

FIG. 5. Numerical primordial amplitude power spectrum at the crossing point for $w = 0.1$ and various values of χ; in that case, $\chi_{\mathrm{F}} = -1.35$ and $\chi_{\mathrm{C}} \simeq 3.86$. From top to bottom: $\chi = 9$, $\chi = \chi_{\mathrm{C}}$ (thick line), $\chi = 2$, $\chi = -0.1$, $\chi = -1.5$ (dashed), and $\chi = -1.3$. This illustrates the fact that although the amplitude depends on χ, the index remains given by (71) provided $\chi \neq \chi_{\mathrm{F}}$ (not shown). For $\chi > \chi_{\mathrm{F}}$, the amplitude is seen to decrease as $\chi \to \chi_{\mathrm{F}}$. It increases again for $\chi < \chi_{\mathrm{F}}$ (the dashed line).

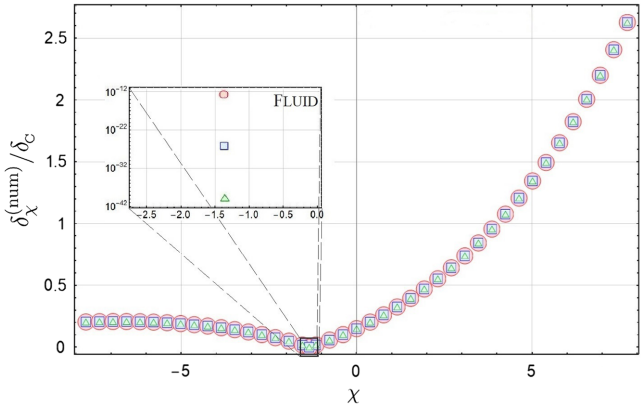

FIG. 6. Ratio $\delta_\chi^{(\mathrm{num})}/\delta_\mathrm{C}$ between the numerical primordial amplitude power spectrum with its analytic counterpart of the conformal parametrization given by Eq. (67) as a function of χ for $w = 0.1$ and three different modes, namely $k_\mathrm{C} = 10^{-15}$ (circles), $k_\mathrm{C} = 10^{-25}$ (squares), and $k = 10^{-35}$ (triangles). The coincidence of the three curves for all values of χ expect χ_F indicates that the spectral index is indeed n_S^C given by (71) and independent of χ. At $\chi = \chi_\mathrm{F} = -1.35$, the zoom shows three distinct points, exhibiting that the spectral index differs, being then given by (70).

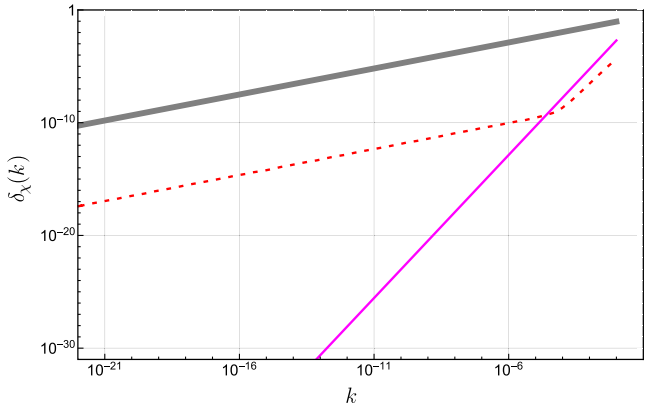

FIG. 7. Primordial density fluctuation spectrum for $w = 0.1$: the conformal case (69) $\chi = \chi_\mathrm{C} = 3.86$ is shown as the thick line above, and the fluid case $\chi = \chi_\mathrm{F}$ as the thin bottom line. The dashed line represents a case close to the fluid case with $\chi = \chi_\mathrm{F} - 10^{-6}$.

we obtain the same power law for the spectral index that in the special case $\chi = \chi_\mathrm{C}$ (71) for all the possible values that χ can take within the conformal parametrization in its generic form (36). In order to clarify this point, we plot, in Fig. 6, the ratio between the numerical spectrum obtained for whatever value of χ and that provided by our analytical approximation (67) for $\chi = \chi_\mathrm{C}$. This plot is but an example for a given value of w, we recovered the same generic image for all values we investigated.

What is also seen in Fig. 6 is a generalization of Fig. 5, namely that the spectral index of scalar perturbations is generically given by (71) except in the case of $\chi = \chi_\mathrm{F}$. The fluid parametrization thus corresponds to the minimum amplitude possible and a different scalar index. In fact, we find that it is understandable as the situation in which the conformal amplitude merely vanishes, leading to the subdominant fluid amplitude being the only one, thereby dominating the full spectrum.

We tested this hypothesis by calculating the spectrum as a function of the wave number for various values of χ close to the fluid case χ_F. The result is illustrated in Fig. 7 in which the power spectrum is calculated numerically for a value of the parameter χ very close to χ_F, superimposed with the analytic solutions for the conformal and the fluid cases. It can be seen that the full spectrum somehow interpolates between both cases, following the fluid power law for large wave numbers and the conformal power law for smaller wave numbers. This suggests that the full spectrum contains both power law terms, the amplitude depending on $\chi - \chi_\mathrm{F}$ for (71): As both power laws are positive, when k decreases, the contribution due to n_S^F becomes smaller compared to that due to n_S^C so the latter finally dominates entirely for very small wave numbers.

B. A sharp transition

A better analytical understanding of the numerical results of the previous section can be achieved by investigating more closely the potential (36) seen as a function of time and χ.

Let us first assume that the reference value for χ is given by the conformal one χ_C. The potential for any value of χ can be written as $V_\chi = V_\mathrm{C} + \delta V$, where

$$\delta V = \frac{2\omega^2}{9Z^4}\frac{1-3w}{(1-w)^2}\delta\chi[1+(\omega\tau)^2]^{-2} \tag{72}$$

and $\delta\chi = \chi - \chi_\mathrm{C}$. Plugging the definition of Z and looking at the large time limit of the full potential, one finds that $\lim_{\omega\tau\to\infty}\delta V \ll \lim_{\omega\tau\to\infty} V_\chi$ so that the main contribution of δV is around the bounce time, namely around $\tau = 0$. As a function of τ, one indeed finds

$$\delta V = \frac{2\omega^2}{9(1+w)^2}\left(\frac{q_\mathrm{B}}{\gamma}\right)^{-4r_\mathrm{F}}\frac{1-3w}{(1-w)^2}\delta\chi[1+(\omega\tau)^2]^{-2r_\mathrm{C}}. \tag{73}$$

Since we focus on the cases $0 \leq w \leq \frac{1}{3}$, one has $\frac{2}{3} \leq r_\mathrm{C} \leq 1$, so that, compared to V_C, one can approximate δV as though its contribution is localized entirely at the bounce; i.e., we replace δV by

$$\delta V_\mathrm{approx} = \Upsilon\delta(\eta), \tag{74}$$

where we assume the coefficient Υ takes the form

$$\Upsilon = \varpi\int_{-\infty}^{\infty}\delta V \mathrm{d}\eta,$$

with $\varpi = \varpi(w) \approx 1$ (we shall evaluate it below), and the integral can be calculated to yield

$$\Upsilon = \frac{2\sqrt{\pi}\omega(1-3w)}{9(1+w)(1-w)^2}\left(\frac{q_{\rm B}}{\gamma}\right)^{-2r_{\rm F}}\frac{\Gamma(r_{\rm C}+\frac{1}{2})}{\Gamma(r_{\rm C}+1)}\varpi(w)\delta\chi, \quad (75)$$

transforming Eq. (56) into

$$\frac{{\rm d}^2 v_k}{{\rm d}\eta^2} - \left[\frac{(q^{r_{\rm C}})''}{q^{r_{\rm C}}} + \Upsilon\delta(\eta)\right]v_k = 0, \quad (76)$$

whose solution is given by Eq. (60) on both sides of the bounce, only with different parameters $A_k^{\rm C<} = A_k^{\rm C}$, $B_k^{\rm C<} = B_k^{\rm C}$ for the contracting phase [given by Eq. (66)] and $A_k^{\rm C>}$, $B_k^{\rm C>}$ for the expanding phases.

Assuming continuity of v_χ at $\eta = 0$ yields $A_k^{\rm C>} = A_k^{\rm C}$, and integrating Eq. (76) around the bounce provides the discontinuity in the time derivative as

$$v_k'(0^+) - v_k'(0^-) = \Upsilon v(0), \quad (77)$$

leading to

$$B_k^{\rm C>} = B_k^{\rm C} - \sqrt{\pi}\frac{\Gamma(r_{\rm C}+\frac{1}{2})}{\Gamma(r_{\rm C}+1)}\frac{\varpi\delta\chi}{\chi_{\rm F}-\chi_{\rm C}}, \quad (78)$$

as can be shown by direct evaluation of $\chi_{\rm F} - \chi_{\rm C}$ as a function of w.

Plugging the above value of $B_k^{\rm C>}$ into the definition (48) and using the mode solution (60), one finds that the power spectrum now consists in two contributions, namely $\delta = k^{3/2}(D+S)$, with the dominant term given by

$$D = \pi|B_k^{\rm C}|\left[1 - \frac{\pi^{3/2}}{4}\frac{\Gamma(r_{\rm C}+\frac{1}{2})}{\Gamma(r_{\rm C}+1)}\frac{\varpi\delta\chi}{\chi_{\rm F}-\chi_{\rm C}}\right], \quad (79)$$

while the subdominant term reads

$$S = S_{\rm N}|C|\left(\frac{q_{\rm B}}{\gamma}\right)^{-\frac{2}{1+3w}}k^{\frac{3(1-w)}{2(1+3w)}}, \quad (80)$$

with normalization

$$S_{\rm N} = \left[1 - \frac{\pi^{3/2}}{2}\frac{\Gamma(r_{\rm C}+\frac{1}{2})}{\Gamma(r_{\rm C}+1)}\frac{\varpi\delta\chi}{\chi_{\rm F}-\chi_{\rm C}}\right]. \quad (81)$$

Note that the two modes are obtained only when one keeps the otherwise negligible contribution in Eq. (66); this is why we kept it in the first place.

Equation (79) shows that, for a fixed unique parameter $\varpi(w)$ of order unity that best approximates $V_{\rm approx}$ to δV, there is one and only one value of χ, for which the dominant mode vanishes, thereby explaining our numerical findings. Therefore, one can assume that the best fit is given by

$$\varpi(w) = \frac{4}{\pi^{3/2}}\frac{\Gamma(r_{\rm C}+1)}{\Gamma(r_{\rm C}+\frac{1}{2})}, \quad (82)$$

leading the dominant term to only vanish for $\chi = \chi_{\rm F}$, in agreement with the above results. For w in our range, this lies between $\varpi(0) \approx 0.7$ and $\varpi(1/3) \approx 0.8$, i.e., a number of order unity as expected.

With the power spectrum (79) vanishing, there remains the subdominant piece, which happens to lead to $\delta \propto k^{n(w,\chi_{\rm F})}$ [see Eq. (70)]. This reproduces exactly the features observed in the previous section and illustrated in Fig. 7, namely that as $\chi \to \chi_{\rm F}$, the dominant amplitude coefficient becomes smaller and smaller and thus comes to actually dominate over the subdominant one only for smaller wave numbers. In the limit $\chi = \chi_{\rm F}$, the coefficient exactly vanishes and the subdominant piece, then being the only one, becomes the only relevant spectrum.

V. CONCLUSION

In this work, we performed a detailed examination of the dynamical ambiguity that naturally arises in models of the primordial universe, in which both the cosmological background and the perturbations are quantized. A previous paper had found that quantizing the background and writing a semiquantum trajectory approximation leads to two different potentials for the perturbations, thereby rendering the theory effectively ambiguous and potentially non predictive.

The model presented in this work is only academic in that it describes a universe whose dynamics is driven by a fluid at all times and fails at reproducing the CMB data: To do so, it would require either $w \sim -2.9 \times 10^{-3}$ for the conformal case and $w \sim -0.988$ in the fluid case. Both being negative, the corresponding models are plagued with incurable instabilities; the model we have discussed here assumes $0 \leq w \leq \frac{1}{3}$ so as to avoid such instabilities. It merely serves as an illustration of the ambiguity and its resolution: One can expect that the same techniques using a scalar field should lead to similar results.

At the classical level, one can build an infinite number of acceptable and equivalent (i.e., related by canonical transformations) perturbation variables which, upon quantization, lead to *a priori* different quantum theories: Obtaining the Mukhanov-Sasaki variable through performing the canonical transformation either before quantization or after the semiquantum trajectory is obtained yields inequivalent potentials, and therefore, one would have guessed, to different predictions for the expected spectrum. We found the astonishing result that despite the presence of a continuous parameter describing the various possible potentials, there are only two possible predictions for the spectral index.

The conformal parametrization reproduces the usual spectrum with $n_{\rm S}^{\rm C}$, the amplitude depending on the parameters of the semiquantum trajectory.

There exists, because of the ambiguity, another possible spectral index, stemming from using the fluid parametrization. We found, however, this prediction to be very special: Within our family of potentials depending on one parameter χ, we found that all values of χ predict the same (conformal) spectral index, except when $\chi \to \chi_{\mathrm{F}}$ exactly, in which case, one gets a different spectrum with no parameter and a single well-defined amplitude.

The fluid case can be explained as leading to the subdominant contribution in the spectrum, the amplitude of the dominant term vanishing for the special value $\chi \to \chi_{\mathrm{F}}$. In that sense, it represents a set of measure zero in the general $\chi \in \mathbb{R}$ so that one can either deduce that the conformal case is the generic, and therefore, the correct one, or, on the contrary, that the fluid case being so special should represent the correct prediction.

The conformal spectrum depends on the ratio between the 3D compact manifold and the observable Universe, as well as on the parameter $\mathfrak{K}$ coming from quantization of the background. There exists some amount of degeneracy between those. The tensor index should be calculated to raise this degeneracy. It is to be expected that a similar behavior will be observed.

In quantum bounce models, the Mukhanov variable belongs to the class of variables that yields the generic prediction for primordial amplitude spectrum. In this sense, its use in semiclassical theories like inflation can be given a deeper justification. On the other hand, it is not the only one in that class. Moreover, which is the most convenient choice of variable depends on the choice of internal time employed in quantization. Hence, the Mukhanov variable constitutes a valid but no longer a preferred choice in quantum bounce models.

ACKNOWLEDGMENTS

P. M. and J. C. M. acknowledge the support of the National Science Centre (NCN, Poland) under the research Grant No. 2018/30/E/ST2/00370.

APPENDIX: QUANTUM CANONICAL TRANSFORMATION

Let us start with the Hamiltonian (13) and implement in a quantum way the canonical transformation taking the fluid variable $\phi_{\boldsymbol{k}}$ into its classical conformal-equivalent $v_{\boldsymbol{k}}$. In what follows, we assume the fields to be real, or more precisely, we focus on the real parts of the fields, the imaginary parts being treated in an exactly similar way so that the full Hamiltonian is merely obtained by adding the real and imaginary components. Besides, for the sake of simplicity, we drop the wave number indices so that our starting point (13) is

$$H_{\phi}^{(2)} = \frac{1}{2}\left[\pi_{\phi}^2 + w(1+w)^2\left(\frac{q}{\gamma}\right)^{4r_{\mathrm{F}}}k^2\phi^2\right], \tag{A1}$$

which is quantized through the replacements $\phi \to \hat{\phi}$, $\pi_{\phi} \to \hat{\pi}_{\phi}$, and $q \to \hat{Q}$, the background Hamiltonian being taken to be $\hat{H}^{(0)} = \frac{1}{2}\hat{P}^2 + K\hat{Q}^{-2}$; that is, we set $\kappa_0 \to \frac{1}{4}$ and $\mathfrak{c}_0 = 2K$ in this appendix; in any case, these variables do not enter in the subsequent results and can therefore be given whichever value to simplify the calculations. As all the variables are now quantum in what follows, we remove all the hats over the operators.

Let us now perform the quantum version of the canonical transformation (17). Switching to a different basis perturbation variable v is achieved by introducing a unitary transformation $U[v(\phi,\pi_{\phi}),\pi_v(\phi,\pi_{\phi})]$ of $\mathcal{H}_{\mathrm{B}} \otimes \mathcal{H}_{\mathrm{P}}$, the Hilbert space of states mixing background and perturbation variables. It can be chosen as

$$U = \mathrm{e}^{i\alpha(Q,P)D_v}\mathrm{e}^{i\beta(Q,P)v^2}, \tag{A2}$$

with $D_v = \frac{1}{2}(v\pi_v + \pi_v v)$ so that $[v, D_v] = iv$; the two Hermitian operators α and β depend only on the background variables Q and P and therefore implicitly on time.

Under the transformation (A2), the field becomes

$$v = U\phi U^{\dagger} \Rightarrow \phi = U^{\dagger}vU = \mathrm{e}^{-\alpha}v + \cdots, \tag{A3}$$

where the ellipsis means higher order terms, which we neglect—in this case, $\mathcal{O}(v^3)$; as a general matter, from that point on, we assume the leading order and do not write explicitly the order of the missing terms.

Similarly, the dilation operator transforms into

$$D_v = UD_{\phi}U^{\dagger} \Rightarrow D_{\phi} = U^{\dagger}D_vU = D_v + 2\beta v^2, \tag{A4}$$

which, given our choice (A2), happens to be exact at all orders. One gets the canonical momentum as

$$\pi_v = \frac{1}{2}\left(D_v v^{-1} + v^{-1}D_v\right),$$

and a similar definition for π_{ϕ} in terms of the equivalent D_{ϕ}. This leads to

$$\pi_{\phi} = \mathrm{e}^{\alpha}\pi_v + \left(\beta\mathrm{e}^{\alpha} + \mathrm{e}^{\alpha}\beta\right)v, \tag{A5}$$

remembering that $[\alpha,\beta] \neq 0$.

The operators ϕ and v obey the usual Heisenberg equation

$$\frac{\mathrm{d}\phi}{\mathrm{d}\tau} = i\left[H_{\phi}^{(2)}(\phi,\pi_{\phi}),\phi\right] \quad \text{and} \quad \frac{\mathrm{d}v}{\mathrm{d}\tau} = i\left[H_{\mathrm{T}}^{(2)}(v,\pi_v),v\right],$$

with the Hamiltonian given by (A1), while its transformed counterpart $H_{\mathrm{T}}^{(2)}(v,\pi_v)$ needs to be determined.

Using (A3) and expanding the time derivative, one gets

$$\frac{\mathrm{d}v}{\mathrm{d}\tau} = i\left[UH_{\phi}^{(2)}U^{\dagger} + iU\frac{\mathrm{d}U^{\dagger}}{\mathrm{d}\tau}, v\right], \tag{A6}$$

thereby defining the transformed Hamiltonian $H_{\mathrm{T}}^{(2)}$. Now, the time derivative of U reads

$$\frac{\mathrm{d}U^{\dagger}}{\mathrm{d}\tau} = i\left[H_{\phi}^{(2)}, U^{\dagger}\right] + \frac{\partial U^{\dagger}}{\partial\tau},$$

so that, from (A6), one gets a cancellation of the first term to yield the total Hamiltonian $H_{\mathrm{T}}^{(2)}(v,\pi_v)$ for the perturbations in terms of the variables v and π_v, namely

$$H_{\mathrm{T}}^{(2)}(v,\pi_v) = iU(v,\pi_v)\dot{U}^{\dagger}(v,\pi_v) + H_{\phi}^{(2)}(U^{\dagger}vU, U^{\dagger}\pi_v U), \tag{A7}$$

a dot meaning partial derivative with respect to the time τ and the last term being calculable from (A1) through the replacements (A3) and (A5).

Expanding (A2) in powers of v and D_v, the first term in (A7) reads

$$iU\dot{U}^{\dagger} = -\dot{\alpha}D_v - (\dot{\beta} + \dot{\alpha}\beta + \beta\dot{\alpha})v^2\cdots. \tag{A8}$$

We now set $\alpha = \alpha(Q) = \ln Z_r$, with Z_r the operator counterpart of (20). The time evolution of α is given by the Heisenberg equation

$$\dot{\alpha} = -i[\alpha, H^{(0)}] = -i\left[\alpha(Q), \frac{1}{2}P^2 + \frac{K}{Q^2}\right], \tag{A9}$$

which yields

$$\underbrace{\frac{\mathrm{d}}{\mathrm{d}\tau}\ln\left[\sqrt{1+w}\left(\frac{Q}{\gamma}\right)^{r}\right]}_{\alpha(Q)} = \dot{\alpha} = \frac{r}{2}\left(iQ^{-2} + 2Q^{-1}P\right), \tag{A10}$$

in which we used $[f(Q), P] = i\mathrm{d}f/\mathrm{d}Q$. This also yields the commutation relation

$$[\dot{\alpha}, \alpha] = -ir^2Q^{-2} = -ir^2\frac{(1+w)^{1/r}}{\gamma^2}\mathrm{e}^{-2\alpha/r} = g(\alpha) \tag{A11}$$

between α and its time derivative.

In order for the transformation (A2) to be canonical, the term proportional to D in the transformed Hamiltonian must disappear. This requires its coefficient to vanish, a condition which is fulfilled provided α and β satisfy

$$\dot{\alpha} = \mathrm{e}^{\alpha}\beta\mathrm{e}^{\alpha} + \frac{1}{2}\left(\mathrm{e}^{2\alpha}\beta + \beta\mathrm{e}^{2\alpha}\right). \tag{A12}$$

Plugging Eq. (A12) into (A11), one gets

$$g(\alpha) = \mathrm{e}^{\alpha}[\beta,\alpha] + \frac{1}{2}\mathrm{e}^{2\alpha}[\beta,\alpha] + \frac{1}{2}[\beta,\alpha]\mathrm{e}^{2\alpha},$$

showing that the commutator $[\alpha,\beta]$ can only depend on α. All terms on the rhs of the above equation commuting, it is easy to solve for the commutator. One gets

$$[\beta,\alpha] = \frac{1}{2}\mathrm{e}^{-2\alpha}g(\alpha) = -\frac{ir(1+w)^{1/r}}{2\gamma^2}\mathrm{e}^{-2\alpha(1+r)/r},$$

so that $\beta = \frac{1}{2}\mathrm{e}^{-2\alpha}\dot{\alpha} + \beta_0(\alpha)$. The function β_0 can be found by replacing the above β into (A12). This yields $\beta_0 = -\frac{1}{2}g(\alpha)\mathrm{e}^{-2\alpha}$, and finally

$$\beta = \frac{1}{2}\mathrm{e}^{-2\alpha}[\dot{\alpha} - g(\alpha)] = -\frac{1}{4}\frac{\mathrm{d}\mathrm{e}^{-2\alpha}}{\mathrm{d}\tau}, \tag{A13}$$

which is expressed in terms of the background operators as

$$\beta = \frac{r}{4(1+w)}\left(\frac{Q}{\gamma}\right)^{-2r}[i(1+2r)Q^{-2} + 2Q^{-1}P]. \tag{A14}$$

One finally gets the Hamiltonian $H_{\mathrm{T}}^{(2)}$, namely

$$H_{\mathrm{T}}^{(2)} = \frac{i}{2}[\beta,\mathrm{e}^{2\alpha}] + \frac{1}{2}\mathrm{e}^{2\alpha}\pi_v^2 + \frac{1}{2}\Bigg[(\beta\mathrm{e}^{\alpha} + \mathrm{e}^{\alpha}\beta)^2 - 2(\dot{\alpha}\beta + \beta\dot{\alpha}) - 2\dot{\beta} + w(1+w)^2\left(\frac{Q}{\gamma}\right)^{4r_{\mathrm{F}}}k^2\mathrm{e}^{-2\alpha}\Bigg]v^2. \tag{A15}$$

The first term in Eq. (A15) depends only on the background variables. It can in fact be evaluated as

$$\frac{i}{2}[\beta,\mathrm{e}^{2\alpha}] = \frac{r^2}{2Q^2},$$

which merely implies a correction to the otherwise unknown parameter K; we neglect this term from now on.

The kinetic term $\propto \pi_v^2$ comes with an overall factor $\frac{1}{2}\mathrm{e}^{2\alpha} = \frac{1}{2}(1+w)(Q/\gamma)^{2r}$, which is exactly of the form obtained in (21), showing that (A2) is indeed the quantum analog of the classical canonical transformation (17) with Z given by (20). Indeed, the wavelength term $\propto k^2$, upon factorizing $\frac{1}{2}(1+w)(Q/\gamma)^{2r}$ appearing in (21), yields exactly the required factor $(Q/\gamma)^{4(r_{\mathrm{F}}-r)}wk^2$ as in (22).

The remaining terms read

$$(\beta e^{\alpha}+e^{\alpha}\beta)^2=\frac{r^2}{1+w}\left(\frac{Q}{\gamma}\right)^{-2r}\left[-\frac{1}{4}(1+r)(5+3r)Q^{-4}+2i(1+r)Q^{-3}P+Q^{-2}P^2\right]$$

and

$$2(\dot{\alpha}\beta+\beta\dot{\alpha})=\frac{r^2}{2(1+w)}\left(\frac{Q}{\gamma}\right)^{-2r}\left[-(4r^2+8r+5)Q^{-4}+8i(1+r)Q^{-3}P+4Q^{-2}P^2\right],$$

which can be directly evaluated using the above expressions, as well as

$$2\dot{\beta}=\frac{r}{1+w}\left(\frac{Q}{\gamma}\right)^{-2r}\left\{\left[2K+\frac{1}{2}(1+r)(1+2r)(3+2r)\right]Q^{-4}-2i(1+r)(1+2r)Q^{-3}P-(1+2r)Q^{-2}P^2\right\},$$

obtained by calculating the commutator of β with the background Hamiltonian.

Finally, the total potential term can be written as

$$\frac{1}{2}(1+w)\left(\frac{Q}{\gamma}\right)^{2r}\left\{\left(\frac{Q}{\gamma}\right)^{4r_{\mathrm{F}}-4r}wk^2+\frac{r(r+1)}{(1+w)^2}\left(\frac{Q}{\gamma}\right)^{-4r}\times Q^{-2}\left[P^2+2i(1+r)Q^{-1}P+g(r)Q^{-2}\right]\right\}v^2, \quad \text{(A16)}$$

where

$$g(r)=-\frac{8K+6+17r+16r^2+3r^3}{4(r+1)}.$$

Comparison with the Hamiltonian (27) reveals that the canonical transformation provides an equivalent result provided the choice $\mathfrak{c}(-2r-2)\to g(r)$ is made, which may not always be possible.

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