Effective constraints and physical coherent states in quantum cosmology: a numerical comparison

Martin Bojowald and Artur Tsobanjan
Institute for Gravitation and the Cosmos, The Pennsylvania State University, 104 Davey Lab, University Park, PA 16802, USA
E-mail: bojowald@gravity.psu.edu and axt236@psu.edu

Received 4 December 2009, in final form 12 April 2010
Published 26 May 2010
Online at stacks.iop.org/CQG/27/145004

Abstract
A cosmological model with a cyclic interpretation is introduced, which is subject to quantum back-reaction and yet can be treated rather completely by physical coherent states as well as effective constraint techniques. By this comparison, the role of quantum back-reaction in quantum cosmology is unambiguously demonstrated. Also the complementary nature of strengths and weaknesses of the two procedures is illustrated. Finally, effective constraint techniques are applied to a more realistic model filled with radiation, a context in which physical coherent states are not available.

PACS numbers: 03.65.Sq, 03.65.Pm, 98.80.Qc
(Some figures in this article are in colour only in the electronic version)

1. Introduction

In order to understand the generic behavior of a quantum system, effective equations\(^1\) are useful. In contrast to individual wavefunctions, or even just stationary states, they directly provide (approximate) equations for time-dependent expectation values. Since the dynamics of expectation values depends on the whole motion of a state—by quantum back-reaction, all moments of a state couple to the expectation values—these equations in general differ from the classical ones by quantum corrections. If quantum corrections, for instance an effective potential, can be found explicitly, an interpretation of quantum dynamics in generic terms becomes much easier. Such results are more general compared to conclusions based on individual states or specific classes of states.

\(^1\) We use the term ‘effective equations’ in a general sense to encompass equations that might follow from an effective action, or be derived in a canonical way. Systematic procedures exist for both ways, and the results agree in cases in which they have been explicitly applied \([1, 2]\).
Especially in quantum cosmology, the ability to draw generic conclusions is important. Not much is known about the state of the universe except, perhaps, that it currently may well be considered semiclassical. But semiclassicality is not a sharp notion, and so wide classes of states, differing for instance by the sizes of their quantum fluctuations or correlations, are still allowed. In any such situation, a generic analysis is called for, most crucially when long-term evolution is involved or when one evolves toward strong-curvature regimes such as the big bang singularity where quantum effects of all kinds are expected to be important.

It is sometimes suggested, at least implicitly (and especially in the context of loop quantization), that quantum cosmology might somehow be different from other quantum systems, and that quantum back-reaction could be ignored in its effective equations. Quantum back-reaction might be weak for certain states or in certain regimes, especially for models close to solvable ones, but this observation cannot be generalized. Like the harmonic oscillator in quantum mechanics, there are harmonic cosmologies where expectation values of states follow exactly the trajectories of a corresponding classical system. Such systems are entirely free of quantum back-reaction. For ‘small anharmonicity’, quantum back-reaction might still be weak, as it is realized in quantum cosmology for matter dominated by its kinetic energy density. But the tough reality of stronger deviations from the solvable ideal of harmonic systems can introduce severe quantum back-reaction, which must be studied in an unbiased and systematic way.

In the present work we demonstrate the effects of quantum back-reaction in two toy models as well as showcase an effective technique for their treatment developed in [6, 7]. Within the first of our models we explicitly compare the effective treatment of constraints to a construction of physical states, briefly discussing the relative strengths of the two approaches. This model is rather simple but, to the best of our knowledge, has not been discussed much yet. It serves to highlight the differences between the kinematical and dynamical properties of semiclassical states for non-harmonic systems.

More specifically, our first model is an anisotropic cosmology of locally rotationally symmetric (LRS) Bianchi I symmetry type, filled with an isotropic, slightly sub-stiff fluid of negative energy density $\rho(a) \propto -\log(a)^2/a^6$ where $a$ is the average scale factor of the anisotropic geometry. With this specific density, the model becomes treatable by physical coherent states, which justifies its contrived and exotic form. Effective constraint techniques [6, 7], applicable much more widely, do not require such a tailored matter source; they are considerably more powerful. As we will see by the explicit comparison of this paper, they capture the information in semiclassical physical states to an excellent degree. Moreover, effective techniques self-consistently determine their ranges of validity. The general applicability of effective constraints will be demonstrated by our final analysis of a model whose matter content, more realistically, is pure radiation.

2. The model

An anisotropic Bianchi I model has a line element

$$\text{d}s^2 = -\text{d}t^2 + \sum_{I=1}^{3} a_I(t)^2 (\text{d}x^I)^2$$

2 A suggestion of this form is made whenever one appeals to exactly solvable models (in this case, an isotropic flat universe sourced by a free, massless scalar) in order to justify the use of similar effective equations in more complicated cases. We note that even in the absence of quantum back-reaction there may still be ‘corrections’ to classical equations of motion if these equations have been modified for other, unrelated reasons. In this paper, we are dealing only with quantum back-reaction.
with three independent scale factors $a_I(t)$ as functions of proper time $t$. For a canonical formulation, we denote the momenta of $h_I := a_I^2$ by $\pi^I$. It is convenient to introduce Misner variables $(\alpha, \beta_+, \beta_-)$ and their momenta $(p_\alpha, p_+, p_-)$ by the canonical transformation \[ \frac{1}{2} \log \left( \frac{h_1}{a_0^2} \right) =: \alpha + \beta_+ + \sqrt{3} \beta_-, \quad 2h_1 \pi^1 :=: \frac{1}{3} p_\alpha + \frac{1}{6} p_+ - \frac{1}{2 \sqrt{3}} p_- \] \[ \frac{1}{2} \log \left( \frac{h_2}{a_0^2} \right) =: \alpha + \beta_+ - \sqrt{3} \beta_-, \quad 2h_2 \pi^2 :=: \frac{1}{3} p_\alpha + \frac{1}{6} p_+ + \frac{1}{2 \sqrt{3}} p_- \] \[ \frac{1}{2} \log \left( \frac{h_3}{a_0^2} \right) =: \alpha - 2 \beta_+ + \sqrt{3} \pi^3 :=: \frac{1}{3} p_\alpha - \frac{1}{3} p_+ \] (1) (2) (3)

In these definitions, $a_0$ is a reference scale factor (e.g. $a_0 = \sqrt{h_1h_2h_3}$ at one moment of time) introduced to be insensitive to coordinate rescalings.

Canonical dynamics in general relativity is determined by the Hamiltonian constraint
\[ C_{\text{grav}} = \frac{\pi_{ab} \pi^{ab} - \frac{1}{4} (\pi^{\alpha\alpha})^2}{\sqrt{\text{det} h}} - \frac{\sqrt{\text{det} h}}{(16\pi G)^2} (3) R = 0 \]
with the spatial metric $h_{ab}$, its Ricci scalar $(3) R$ and its momenta $\pi^{ab}$. Reduced to Bianchi I metrics in Misner variables, specified to a lapse function $N = \sqrt{\text{det} h} = a_1 a_2 a_3$, it simplifies considerably to the form
\[ C_{\text{Bianchi I}} = \frac{1}{2} \left( p_\alpha^2 + p_+^2 + p_-^2 \right). \]
(4) (5)

As one can check directly, the constraint generates the correct Hamiltonian equations of motion in coordinate time, from which the Kasner solutions follow.

We now restrict the model further by requiring the anisotropy parameter $\beta_-$ and its momentum $p_-$ to vanish: $\beta_- = 0 = p_-$. In this way, which can easily be confirmed to be consistent with the equations of motion, we enhance the symmetry and leave two independent gravitational variables: the logarithm of the average scale factor $\alpha$ and one anisotropy parameter $\beta_+$. The resulting Hamiltonian constraint is equivalent to that of a free massless relativistic particle.

To introduce a ‘potential’, we will work with a matter source whose energy density is
\[ \rho = -\rho_0 \log a_0^2 = -\rho_0 a_0^6 e^{-2\alpha}. \]
(6)

where, in addition to $a_0$ already introduced, $\rho_0$ is the matter energy density at some ‘initial’ time. In the presence of matter, its density multiplied with $a^6$ is to be added to the constraint (5). It becomes
\[ C_{\text{LRS}} = -p_\alpha^2 + p_+^2 - \alpha^2 \nu \]
(7)

if we make convenient (and irrelevant) choices for the prefactors and define $\nu = \rho_0 a_0^6$. Our constraint then becomes that of a ‘relativistic harmonic oscillator’ as studied in [7]:
\[ p_\alpha^2 = p_+^2 + \nu \alpha^2. \]
(8)

In this analogy, we consider $\beta_+$ as our time variable, and $p_+$ as the corresponding ‘energy.’ Evolution of $\alpha$ and $p_\alpha$ with respect to $\beta_+$ is then generated by the Hamiltonian
\[ p_\alpha = \pm \sqrt{p_+^2 + \nu \alpha^2}. \]

A more realistic matter content could be chosen as radiation, with an energy density $\rho \propto a^{-4} = e^{-4\alpha}$. Here, the Hamiltonian is $p_+ = \pm \sqrt{p_\alpha^2 + \nu e^{2\alpha}}$.

3 If we introduce a finite region of coordinate size $V_0$ to integrate out homogeneous quantities such as the symplectic form $\int \delta x \delta b_{ab} \wedge \delta \pi^m = V_0 b_0 h_1 \wedge \delta \pi^f = b h_1 \wedge \delta \pi^f$, the momenta $\pi^f = V_0 \tilde{\pi}^f$ depend on the rather arbitrary $V_0$. The lapse function as chosen here would then be homogeneous in $V_0$, as well, such that $V_0^2 a^6 \rho$ is the matter contribution to the constraint. With this, all its terms scale in the same way if $V_0$ is changed. Solving the constrained system, we obtain the same reduced phase space for all choices of $V_0$. 

2.1. Classical behavior

We define \( H = \sqrt{p_\alpha^2 + \nu \alpha^2} \), such that our constraint solved for \( p_\alpha \) takes the deparametrized form

\[
C_{\text{deparametrized}} = p_\alpha \pm H(\alpha, p_\alpha) = 0.
\]

(From now on we choose \( p_\alpha \) positive, to be specific.) This constraint generates Hamiltonian equations of motion for the anisotropies \( p_\alpha = 0 \) and \( \beta_\alpha = 1 \), allowing us to identify the time parameter along its flow with \( \beta_\alpha \) as an internal time. All derivatives in Hamiltonian equations of motion are then with respect to \( \beta_\alpha \), specifically

\[
\frac{\mathrm{d} \alpha}{\mathrm{d} \beta_\alpha} = [\alpha, H] = \frac{p_\alpha}{H}, \quad \frac{\mathrm{d} p_\alpha}{\mathrm{d} \beta_\alpha} = [p_\alpha, H] = -\frac{\nu \alpha}{H}.
\]

Since \( H = \mp p_\alpha \) is constant in \( \beta_\alpha \), we can combine these equations to a second-order one for \( \alpha(\beta_\alpha) \), \( d^2 \alpha / d \beta_\alpha^2 = -\nu \alpha / H^2 \) solved by

\[
\alpha(\beta_\alpha) = A \sin(\beta_\alpha \sqrt{\nu / H}) + B \cos(\beta_\alpha \sqrt{\nu / H}) \tag{9}
\]

with integration constants \( A \) and \( B \). The equation of motion for \( \alpha_+ \) shows that

\[
p_{\alpha_+}(\beta_\alpha) = \sqrt{\nu}(A \cos(\beta_\alpha \sqrt{\nu / H}) - B \sin(\beta_\alpha \sqrt{\nu / H})). \tag{10}
\]

With this, the integration constants can be related to \( H \) by \( H^2 = \nu(A^2 + B^2) \). Solutions in phase space are ellipses of axis lengths \( H = |p_\alpha| \) and \( \sqrt{\nu} \), traversed in time \( \beta_\alpha \) with frequency \( (2\pi H / \sqrt{\nu})^{-1} \).

To derive the behavior with respect to proper time, we use the original constraint \( C_{\text{LRS}} \) not yet deparametrized, and recall that we chose a lapse function \( N = a_1 a_2 a_3 = a_0^3 \exp(3\nu) \). Thus, the equation of motion for \( \beta_\alpha \) with respect to proper time \( \tau \) is

\[
\frac{\mathrm{d} \beta_\alpha}{\mathrm{d} \tau} = \{\beta_\alpha, \exp(3\nu C_{\text{LRS}})\} = 2 e^{-3\nu} p_\alpha a_0^{-3}. \tag{11}
\]

From here, we determine proper time as a function of \( \beta_\alpha \) by integrating

\[
\tau = \frac{a_0^3}{2 p_\alpha} \int e^{3\nu(\beta_\alpha)} \, \mathrm{d} \beta_\alpha
\]

with our solution \( \alpha(\beta_\alpha) \). Inverting the solution allows us to insert \( \beta_\alpha(\tau) \) into \( \alpha(\beta_\alpha) \) and \( p_\alpha(\beta_\alpha) \), resulting in solutions as functions of proper time.

It is not easy to integrate \( \tau(\beta_\alpha) \) explicitly, but it is clear from the integrand that \( \tau(\beta_\alpha) \) is a monotonic, one-to-one function which can be inverted globally. Thus, \( \alpha(\tau) \) and \( p_\alpha(\tau) \) are defined and finite for all values of proper time. There is no singularity in this model. Clearly, the negative amount of matter energy violates energy conditions sufficiently strongly to provide the cyclic bouncing solutions embodied by ellipses in the \((\alpha, p_\alpha)\)-plane.

One can see this directly from the Friedmann-type equation resulting from the Hamiltonian constraint. We have \( \dot{p}_\alpha^2 = p_\alpha^2 - \nu \alpha^2 \), where \( p_\alpha \) is a constant and \( p_\alpha \) can be obtained from the equation \( \frac{\mathrm{d} \alpha}{\mathrm{d} \tau} = \left\{ \alpha, a_0^{-3} e^{3\nu} C_{\text{LRS}} \right\} = -2a_0^{-3} e^{-3\nu} p_\alpha \), relating it to the derivative of \( \alpha \) by proper time \( \tau \). Thus, the constraint equation reads

\[
\frac{1}{4} a_0^6 e^{6\alpha} \left( \frac{\mathrm{d} \alpha}{\mathrm{d} \tau} \right)^2 - \frac{4}{a_0^6 e^{6\alpha}} (p_\alpha^2 - \nu \alpha^2) = 0
\]

and for \( a = a_0 \exp(\alpha) \) implies

\[
\left( \frac{\dot{a}}{a} \right)^2 = 4 p_\alpha^2 - 4 p_0 (\log a/a_0)^2 \left( a/a_0 \right)^6. \tag{12}
\]
On the right-hand side, we identify \( 4p_c^2/a^6 \) as the anisotropic shear term and the contribution \(-4p_4a_0^2(log a/a_0)^2/a^6 \) as our exotic energy density.

The Friedmann equation shows when \( a \) can vanish, which is realized for \( log a/a_0 = \pm p_s/\sqrt{v} \), two solutions which correspond to the maximal and minimal \( \alpha \) along our circles. The extrema indeed give us a maximum for \( log a/a_0 = p_s/\sqrt{v} \) and a minimum for \( log a/a_0 = -p_s/\sqrt{v} \). The sign of \( \dot{a} \), by the Raychaudhuri equation, is determined by the sign of \( \rho + 3P \) of all the matter sources combined. Here, pressure is obtained from the energy density as the negative derivative of energy by volume, i.e. by

\[
P = -\frac{\partial E}{\partial V} = -\frac{d(a^3 \rho(a))}{3a^2 da}
\]

resulting in \( P_{\text{neg}} = \rho_{\text{neg}}(1 - \frac{2}{3}(log a/a_0)^{-1}) \) for the negative energy fluid with \( \rho_{\text{neg}} = -4v(log a/a_0)^2/a^6 \), and \( P_{\text{shear}} = \rho_{\text{shear}} \) for the shear contribution with \( \rho_{\text{shear}} = 4p_c^2/a^6 \). For \( \rho + 3P \), this gives

\[
\rho + 3P = \rho_{\text{neg}} \left( 4 - \frac{2}{log(a/a_0)} \right) + 4\rho_{\text{shear}}
\]

which at the extrema \( log a/a_0 = \pm p_s/\sqrt{v} \) evaluates to \( \pm 8\sqrt{v}p_s/a^6 \). The extrema provide a maximum at \( log a/a_0 = p_s/\sqrt{v} \) and a minimum at \( log a/a_0 = -p_s/\sqrt{v} \), and the evolution is that of a cyclic model with infinitely many bounces and recollapses.

For the model with radiation, we have equations of motion \( d\alpha/d\beta_+ = p_\alpha/H \) and \( d\rho_\alpha/d\beta_+ = v \dot{\alpha}/H \), with \( H \) still a constant. The second-order equation for \( \alpha(\beta_+) \) becomes \( d^2\alpha/d\beta^2_+ = v \dot{\alpha}/H^2 \). For the solution of this model, see section 4.

2.2. Quantum representation

To represent the model as a quantum system, we start with the obvious kinematical Hilbert space \( L^2(\mathbb{R}^2, d\alpha d\beta_+) \) of square integrable wavefunctions of two variables \( \beta_+ \) and \( \alpha \). The momentum operators are derivatives times\( \hbar \), as usual. To arrive at observable information and physical states, we have to implement the constraint operator

\[
\hat{C} = \hat{p}^2_\alpha - \hat{\alpha}^2 = -\hbar^2 \frac{\partial^2}{\partial \alpha^2} + \hbar^2 \frac{\partial^2}{\partial \beta^2_+} - \alpha^2,
\]

find its kernel and equip it with a physical inner product.

To analyze the quantum constraint, we reformulate it in a first-order way in our time variable \( \beta_+ \) by taking a square root:

\[
\frac{\hbar}{i} \frac{\partial}{\partial \beta_+} \Psi(\alpha, \beta_+) = \pm \left( \hat{p}^2_\alpha + \hat{\alpha}^2 \right)^{1/2} \Psi(\alpha, \beta_+) =: \pm \hat{H} \Psi(\alpha, \beta_+),
\]

introducing the deparametrized Hamiltonian operator \( \hat{H} = (\hat{p}^2_\alpha + \hat{\alpha}^2)^{1/2} \). All solutions of this equation can be expressed as

\[
\Psi_\pm(\alpha, \beta_+) = \sum_{n=0}^{\infty} c_n \varphi_n(\alpha) \exp(\mp i\lambda_n \beta_+/\hbar)
\]

where \( \varphi_n \) are the eigenstates of \( \hat{H} \) with eigenvalues \( \lambda_n \), normalized as usual

\[
\int_{-\infty}^{\infty} d\alpha \varphi_n(\alpha) \varphi_m(\alpha) = \delta_{nm}.
\]

Since \( \hat{H} \) is the square root of the (positive definite) harmonic

\[
\text{Henceforth, for this model, we drop } v \text{ for simplicity. It can be absorbed into the variables by first dividing the constraint throughout by } \sqrt{\gamma}, \text{ followed by the canonical transformation } \alpha' = v^{1/4} \alpha, \ p'_\alpha = v^{-3/4} p_\alpha, \ \beta'_+ = v^{1/4} \beta_+, \ p'_s = v^{-1/4} p_s,
\]

\[
5
\]
oscillator Hamiltonian (with ‘mass’ \( m = 1/2 \) and ‘frequency’ \( \omega = 2 \)), its eigenstates are of the well-known form, with eigenvalues \( \lambda_n = \sqrt{(2n + 1)\hbar} \).

In (16), the subscript \( \pm \) indicates the sign taken when solving for \( p_+ \) by a square root. Solutions naturally split into two classes, positive-frequency solutions \( \Psi_+ \) and negative-frequency solutions \( \Psi_- \). The separation into two classes becomes relevant when we introduce the inner product

\[
(\Psi, \Phi)_{\text{aux}} := i\hbar \int_{-\infty}^{\infty} d\alpha \left( \Psi^*(\alpha, \beta_+) \frac{\partial}{\partial \beta_+} \Phi(\alpha, \beta_+) - \Phi(\alpha, \beta_+) \frac{\partial}{\partial \beta_+} \Psi^*(\alpha, \beta_+) \right)
\]

of the Klein–Gordon form. Although \( \beta_+ \) appears on the right-hand side, the inner product evaluated on solutions (16) is time independent. However, \((\cdot, \cdot)_{\text{aux}}\) is not positive definite: it is positive for positive-frequency solutions, but negative for negative-frequency solutions. A positive-frequency solution is automatically orthogonal to a solution with the sign of its frequency flipped. To correct the sign, we define the physical inner product as

\[
\langle \Psi, \Phi \rangle := \begin{cases} 
(\Psi, \Phi)_{\text{aux}} & \text{if } \Psi \text{ and } \Phi \text{ are positive frequency} \\
-(\Psi, \Phi)_{\text{aux}} & \text{if } \Psi \text{ and } \Phi \text{ are negative frequency} \\
0 & \text{otherwise}
\end{cases}
\]

and extend it linearly to superpositions of positive- and negative-frequency solutions. (Alternatively, we may declare positive- and negative-frequency solutions, respectively, to define two superselection sectors. The procedure here is analogous to [9].) This completes the construction of the physical Hilbert space.

The square magnitude of the wavefunction in (16) does not represent the probability distribution of finding the system at a particular value of \( \alpha \) for a fixed \( \beta_+ \) due to the specific form of the inner product (17). Following constructions of states for relativistic particles (see e.g. [10]), we define a ‘Newton–Wigner wavefunction’ [11] as

\[
\Psi_{NW}(\alpha, \beta_+) = \sum_{n=0}^{\infty} \tilde{c}_n \varphi_n(\alpha) \exp(\mp i\lambda_n \beta_+ / \hbar),
\]

where \( \tilde{c}_n = c_n / \sqrt{2\lambda_n} \). It is straightforward to verify that, when restricted to positive- or negative-frequency solutions, the scalar product (18) in this representation takes the form

\[
\langle \Psi, \Phi \rangle = \int_{-\infty}^{\infty} d\alpha \Psi_{NW}^*(\alpha, \beta_+) \Phi_{NW}(\alpha, \beta_+).
\]

The square magnitude of the ‘Newton–Wigner wavefunction’ does represent localization in the spectrum of \( \hat{a} \) as defined through the ladder operators below. For the purposes of computing expectation values of observables it is, of course, irrelevant which representation we choose.

From physical states, \( \beta_+ \)-dependent expectation values (or moments) can be computed, playing the role of evolving observables. As with the non-relativistic harmonic oscillator, this is most easily done using ladder operators: \( \hat{a} = \sqrt{\hbar/2}(\hat{a}^\dagger + \hat{\alpha}) \), \( \hat{p}_\alpha = i\sqrt{\hbar/2}(\hat{a}^\dagger - \hat{\alpha}) \). A direct calculation gives

\[
\langle \Psi_+, \hat{a} \Psi_+ \rangle(\beta_+) = \sum_{n=0}^{\infty} \sqrt{2\hbar(n + 1)} \Re(\tilde{c}_n^* \tilde{c}_{n+1} \exp(-i\beta_+(\lambda_{n+1} - \lambda_n)/\hbar))
\]

(20)

\[
\langle \Psi_+, \hat{p}_\alpha \Psi_+ \rangle(\beta_+) = \sum_{n=0}^{\infty} \sqrt{2\hbar(n + 1)} \Im(\tilde{c}_n^* \tilde{c}_{n+1} \exp(-i\beta_+(\lambda_{n+1} - \lambda_n)/\hbar))
\]

(21)

and similarly for moments.
Physical Hilbert spaces can be constructed and physical states decomposed in this way whenever one knows an explicit diagonalization of the Hamiltonian $\hat{H}$. For our model, the closeness to the harmonic oscillator has an additional advantage in that it allows us to use its simple form of coherent states—Gaussians of arbitrary width expanded in the stationary states—as initial values for evolution in $\beta_+$. For the non-relativistic harmonic oscillator, the resulting physical states would be dynamical coherent states: their shape would remain unchanged and they keep saturating the uncertainty relation at all times. Moreover, their expectation values follow the classical trajectories exactly, without quantum back-reaction. For the relativistic harmonic oscillator, and thus our anisotropic toy model, the dynamical behavior of the states is still to be seen. We thus assume an initial state, at some fixed value of $\beta_+$, of the kinematical coherent form

$$\tilde{c}_n = \exp \left( -\frac{|z|^2}{2} \right) \frac{z^n}{\sqrt{n!}}, \quad z \in \mathbb{C}$$

such that $\Psi^{NW}(\alpha, 0) = (2/\pi)^{1/4} \exp \left( -\frac{1}{2}(|z|^2 - z^2 + 2\alpha^2 - 4iz\alpha) \right)$ from (19). A time-dependent physical state then has coefficients

$$\tilde{c}_n e^{-i\alpha_n \beta_+ \hbar} = \frac{1}{\sqrt{n!}} e^{-|z|^2/2} z^n e^{-i\sqrt{2n+1}\beta_+ / \hbar}$$

in its expansion by the $\varphi_n(\alpha)$. With the square root of $2n + 1$, the exponentials cannot simply be combined to a $\beta_+$-dependent $z(\beta_+)^n$. The shape of the state changes as $\beta_+$ moves away from zero: the time-dependent coefficients are no longer of the form (22) for $\beta_+ \neq 0$. Physical states with initial conditions given by the coherent states of the non-relativistic harmonic oscillator are not dynamical coherent states. The model introduced here does show spreading and quantum back-reaction, which makes it interesting for a comparison with effective constraint techniques.

2.3. Effective constraints

In an effective treatment of a quantum system, we can consider the same dynamics, but focus on the algebra of observables. Results will thus be manifestly representation independent. To set up this framework, no approximations are required; we are thus dealing with an exact quantum theory. Only when evaluating the equations, which would give us expressions such as $\langle \hat{a} \rangle(\beta_+)$ or moments of a state as functions of $\beta_+$, do approximation schemes typically enter. This is no different to a representation-based treatment, where exact evaluations of expectation values such as (20) or (21) are difficult to sum explicitly.

At the kinematical level, effective techniques are based entirely on the algebra of basic operators, in our case $[\hat{\beta}_+, \hat{\beta}_-] = i\hbar$ and $[\hat{a}, \hat{a}_n] = i\hbar$, with all other basic commutators vanishing. As it happens at the quantum level, dynamics is brought in by a constraint operator $\hat{C}$ which might have more complicated algebraic relationships with the basic operators, no longer forming a closed algebra.

A whole representation of these algebraic relationships on wavefunctions carries much more details than necessary for extracting physical results. Instead, it is often convenient to focus directly on expectation values and derive dynamical equations for them, avoiding the detour of computing wavefunctions. Expectation values are not sufficient to characterize a state or its dynamics, but when combined with all moments

$$\Delta(O_1 \ldots O_n) := \left( \prod_{i=1}^{n} (\hat{O}_i - \langle \hat{O}_i \rangle) \right)_{\text{Weyl}}$$

(23)
well defined at least for a dense set of states, a complete set of variables results. Here, the subscript ‘Weyl’ in the definition of the moments indicates that we are ordering all operator products totally symmetrically. Any of the basic operators, $\hat{p}_x$, $\hat{p}_y$, $\hat{a}$ and $\hat{p}_\alpha$, can appear as the $\hat{O}_i$ in the basic moments. (To match with the standard notation, we will write $\Delta (O^2) = \langle \Delta O \rangle^2$ for fluctuations.)

Expectation values of basic operators together with the moments can be used to characterize an arbitrary state (pure or mixed); they can be used as coordinates on the state space. Moreover, the commutator of basic operators endows the state space with a Poisson structure, defined by

$$\{\langle \hat{A} \rangle, \langle \hat{B} \rangle \} := \frac{\langle [\hat{A}, \hat{B}] \rangle}{\hbar} \quad (24)$$

for any operators $\hat{A}$ and $\hat{B}$. By linearity and the Leibniz rule, this defines Poisson brackets between all the moments and expectation values. In this way, the quantum phase space is defined. It is not a linear space since there are restrictions for the moments, most importantly the uncertainty relations such as

$$\left(\Delta a^2\right)\left(\Delta p_\alpha\right)^2 - \left(\Delta (a p_\alpha)\right)^2 \geq \hbar^2/4 \quad (25)$$

On this kinematical quantum phase space, the constraint $\hat{C}$ must be imposed. For a constraint operator polynomial in the basic operators,

$$C_{\text{pol}} := \langle \hat{C}_{\text{pol}} - \langle \hat{C}_{\text{pol}} \rangle \hat{C} \rangle \quad (26)$$

defines a function on the state space, expandable in the moments, for any arbitrary polynomial $\hat{C}_{\text{pol}}$ of the basic operators. This infinite set of functions satisfies two important properties: (i) all these functions vanish on physical states annihilated by $\hat{C}$, and (ii) they form a first-class set in the sense of classical constraint analysis, i.e. $\{C_{\text{pol}}, C_{\text{pol}}'\}$ vanishes on the subset of the phase space where all $C_{\text{pol}}$ vanish. The quantum constraint $\hat{C}$ can thus be implemented on the space of moments by imposing the infinite set $\{C_{\text{pol}}\}$ as constraints as one would do it on a classical phase space. We have to find the submanifold on which all constraints vanish and factor out the flow generated by them. If this reduction is completed, we obtain the physical quantum phase space and can look for solutions of observables.

This procedure has several advantages [6]. As already mentioned, it is completely representation independent and instead focuses on algebraic aspects of a quantum system. As a consequence, it works equally well for constraint operators with zero in their continuous spectra and those with zero in their discrete spectrum. Any difficulties in finding physical inner products can be avoided, for the physical normalization arises automatically when the constraints are solved for moments.

Once we try to find specific solutions, there are of course practical difficulties. We are dealing with infinitely many constraints on an infinite-dimensional phase space. Sometimes, this set of equations decouples to finitely many ones, but this happens only in rare solvable cases. In more general systems, we must use approximations to reduce the set to a finite one of relevant equations, with a semiclassical approximation as the main example. Here, we look...
for solutions whose moments satisfy a certain hierarchy, higher moments in the semiclassical case being suppressed by powers of \( \hbar \). To any given order in \( \hbar \), only a finite number of moments need to be considered, subject to a finite number of non-trivial constraints.

In order to perform such a truncation we first need to re-express conditions stemming from (26) in terms of the expectation values and moments of (23); subsequently, moments above some chosen order will be discarded. In our model, for example, one of the constraint conditions to be enforced is \( C_α := \langle (\hat{a} - \langle \hat{a} \rangle)\hat{C} \rangle = 0 \). Here we are dealing with low-order polynomials and the corresponding condition on expectation values and moments is straightforward to derive explicitly:

\[
C_α = \langle (\hat{a} - \langle \hat{a} \rangle)\left( \hat{p}_a^2 - \hat{p}_a^2 - \hat{a}^2 \right) \rangle = \langle (\hat{a} - \langle \hat{a} \rangle)\hat{p}_a^2 \rangle - \langle (\hat{a} - \langle \hat{a} \rangle)\hat{p}_a^2 \rangle - \langle (\hat{a} - \langle \hat{a} \rangle)\hat{a}^2 \rangle.
\]

In each of the terms in the last expression, one needs to replace powers of observables with corresponding powers of \( (\hat{O} - \langle \hat{O} \rangle) \). For example, the middle term can be rewritten as

\[
\langle (\hat{a} - \langle \hat{a} \rangle)\hat{p}_a^2 \rangle = \langle (\hat{a} - \langle \hat{a} \rangle)(\hat{p}_a - \langle \hat{p}_a \rangle)^2 \rangle + 2\langle \hat{p}_a \rangle\langle (\hat{a} - \langle \hat{a} \rangle)(\hat{p}_a - \langle \hat{p}_a \rangle) \rangle + \langle \hat{p}_a \rangle^2\langle \hat{a} - \langle \hat{a} \rangle \rangle,
\]

where the last term vanishes as \( \langle (\hat{a} - \langle \hat{a} \rangle) \rangle = \langle \hat{a} \rangle - \langle \hat{a} \rangle = 0 \). The remaining terms need to be ordered symmetrically in order to write them in terms of moments as in (23), which can be accomplished with the use of the canonical commutation relations. Continuing with the example, the above term becomes

\[
\langle (\hat{a} - \langle \hat{a} \rangle)\hat{p}_a^2 \rangle = \langle (\hat{a} - \langle \hat{a} \rangle)(\hat{p}_a - \langle \hat{p}_a \rangle)^2 \rangle \text{Weyl} + \langle \hat{p}_a \rangle(2\langle (\hat{a} - \langle \hat{a} \rangle)(\hat{p}_a - \langle \hat{p}_a \rangle) \rangle \text{Weyl} + \hat{h}]
\]

with

\[
\langle (\hat{a} - \langle \hat{a} \rangle)(\hat{p}_a - \langle \hat{p}_a \rangle)^2 \rangle \text{Weyl} = \frac{1}{2}\langle (\hat{a} - \langle \hat{a} \rangle)(\hat{p}_a - \langle \hat{p}_a \rangle)^2 \rangle + \langle \hat{p}_a \rangle(\langle (\hat{a} - \langle \hat{a} \rangle)(\hat{p}_a - \langle \hat{p}_a \rangle) \rangle + \langle \hat{p}_a - \langle \hat{p}_a \rangle \rangle^2(\hat{a} - \langle \hat{a} \rangle)).
\]

Proceeding in this way one can write the constraint condition using moments as

\[
C_α = 2\langle \hat{p}_a \rangle\Delta(p_α, α) - 2\langle \hat{p}_a \rangle\Delta(αp_α) - 2\langle \hat{a} \rangle(\Deltaα)\hat{a}^2 + \Delta(αp_α^2) + Δ(α^2).
\]

If we are interested only in the leading order quantum dynamics corrections to the classical equations of motion we truncate at order \( \hbar \), which corresponds to discarding the third-order moments in the expression above. Performing this truncation consistently for all constraint conditions for our model we are left with only five non-trivial constraints

\[
C = \langle \hat{p}_a \rangle^2 - \langle \hat{p}_a \rangle^2 - \langle \hat{a} \rangle^2 + (\Delta p_α)^2 - (\Delta p_α)^2 - (\Delta α)^2 = 0 \tag{27}
\]

\[
C_β_a = 2\langle \hat{p}_a \rangle\Delta(β_a, p_α) + \hat{h}\langle \hat{p}_a \rangle - 2\langle \hat{p}_a \rangle\Delta(β_a, p_α) - 2\langle \hat{a} \rangle\Delta(β_α, α) = 0 \tag{28}
\]

\[
C_ρ_a = 2\langle \hat{p}_a \rangle\Delta(p_α, α) - 2\langle \hat{p}_a \rangle\Delta(p_α, α) - 2\langle \hat{a} \rangle\Delta(αp_α) + \hat{h}\langle \hat{p}_a \rangle - 2\langle \hat{a} \rangle(\Deltaα)^2 = 0 \tag{29}
\]

\[
C_μ_a = 2\langle \hat{p}_a \rangle\Delta(p_α, α) - 2\langle \hat{p}_a \rangle\Delta(αp_α) - \hat{h}\langle \hat{p}_a \rangle - 2\langle \hat{a} \rangle\Delta(α^2) = 0 \tag{30}
\]

\[
C_ρ_a = 2\langle \hat{p}_a \rangle\Delta(p_α, α) - 2\langle \hat{p}_a \rangle\Delta(αp_α) - 2\langle \hat{a} \rangle\Delta(αp_α) + \hat{h}\langle \hat{a} \rangle = 0. \tag{31}
\]
is equivalent to a deparametrized quantum system with the constraint \( C_Q = \langle \hat{p}_u \rangle \pm H_Q \) with the reduced Hamiltonian

\[
H_Q = \sqrt{\langle \hat{p}_u \rangle^2 + \langle \hat{a} \rangle^2} \left( 1 + \frac{\langle \hat{a} \rangle^2 (\Delta p_u)^2 - 2 \langle \hat{a} \rangle \langle \Delta p_u \rangle \Delta (\alpha p_u) + \langle \hat{p}_u \rangle^2 (\Delta \alpha)^2}{2 (\langle \hat{p}_u \rangle^2 + \langle \hat{a} \rangle^2)^2} \right) + O((\Delta p_u)^4) + O((\Delta \alpha)^4) + O((\Delta (\alpha p_u))^2). \tag{32}
\]

To the leading order, we reproduce the classical Hamiltonian, but there are corrections from quantum fluctuations and correlations coupling to the expectation values. Moreover, from the Poisson brackets between moments, we obtain Hamiltonian equations of motion showing us how a state spreads or is being squeezed. We have

\[
\frac{d\langle \hat{a} \rangle}{d\beta_\epsilon} = \frac{\langle \hat{p}_u \rangle}{\sqrt{\langle \hat{p}_u \rangle^2 + \langle \hat{a} \rangle^2}} \left( \langle \hat{p}_u \rangle (\Delta \alpha)^2 (2 \langle \hat{a} \rangle^2 - \langle \hat{a} \rangle^2) + \langle \hat{a} \rangle \Delta (\alpha p_u) (4 \langle \hat{p}_u \rangle^2 - 2 \langle \hat{a} \rangle^2) - 3 \langle \hat{p}_u \rangle \langle \hat{a} \rangle (\Delta p_u)^2 \right) - \frac{3 \langle \hat{a} \rangle (\Delta p_u)^2 (\Delta \alpha)^2 - \langle \hat{p}_u \rangle \Delta (\alpha p_u) (4 \langle \hat{p}_u \rangle^2 - 2 \langle \hat{a} \rangle^2) - \langle \hat{a} \rangle (\Delta p_u)^2 (2 \langle \hat{p}_u \rangle^2 - \langle \hat{a} \rangle^2)}{2 (\langle \hat{p}_u \rangle^2 + \langle \hat{a} \rangle^2)^2}. \tag{34}
\]

\[
\frac{d\langle \hat{p}_u \rangle}{d\beta_\epsilon} = -\frac{\langle \hat{a} \rangle}{\sqrt{\langle \hat{p}_u \rangle^2 + \langle \hat{a} \rangle^2}} \left( \langle \hat{p}_u \rangle (\Delta \alpha)^2 (2 \langle \hat{a} \rangle^2 - \langle \hat{a} \rangle^2) + \langle \hat{a} \rangle \Delta (\alpha p_u) (4 \langle \hat{p}_u \rangle^2 - 2 \langle \hat{a} \rangle^2) - 3 \langle \hat{p}_u \rangle \langle \hat{a} \rangle (\Delta p_u)^2 \right) - \frac{3 \langle \hat{a} \rangle (\Delta p_u)^2 (\Delta \alpha)^2 - \langle \hat{p}_u \rangle \Delta (\alpha p_u) (4 \langle \hat{p}_u \rangle^2 - 2 \langle \hat{a} \rangle^2) - \langle \hat{a} \rangle (\Delta p_u)^2 (2 \langle \hat{p}_u \rangle^2 - \langle \hat{a} \rangle^2)}{2 (\langle \hat{p}_u \rangle^2 + \langle \hat{a} \rangle^2)^2}. \tag{35}
\]

\[
\frac{d(\Delta \alpha)^2}{d\beta_\epsilon} = \frac{2 (\langle \hat{a} \rangle^2 \Delta (\alpha p_u) - 2 \langle \hat{a} \rangle \langle \Delta p_u \rangle \Delta \alpha)^2}{\langle \langle \hat{p}_u \rangle^2 + \langle \hat{a} \rangle^2 \rangle^2}. \tag{36}
\]

\[
\frac{d(\Delta p_u)^2}{d\beta_\epsilon} = \frac{2 \langle \hat{a} \rangle \langle \Delta p_u \rangle^2 - 2 \langle \hat{a} \rangle^2 \Delta (\alpha p_u)}{\langle \langle \hat{p}_u \rangle^2 + \langle \hat{a} \rangle^2 \rangle^2}. \tag{37}
\]

\[
\frac{d\Delta (\alpha p_u)}{d\beta_\epsilon} = \frac{\langle \hat{a} \rangle^2 (\Delta p_u)^2 - \langle \hat{p}_u \rangle^2 (\Delta \alpha)^2}{\langle \langle \hat{p}_u \rangle^2 + \langle \hat{a} \rangle^2 \rangle^2}. \tag{38}
\]

Solutions \( \langle \hat{a} \rangle(\beta_\epsilon), \langle \hat{p}_u \rangle(\beta_\epsilon), (\Delta \alpha)^2(\beta_\epsilon), (\Delta p_u)^2(\beta_\epsilon), \) and \( \Delta (\alpha p_u)(\beta_\epsilon) \) provide physical observables, corresponding to expectation values and moments in physical states, showing us how a state moves and spreads.

3. Comparison

Initially, the kinematical coherent state with expansion coefficients given by (22) yields the expectation values \( \langle \hat{a} \rangle|_{t=0} = \text{Re}(z) \) and \( \langle \hat{p}_u \rangle|_{t=0} = \text{Im}(z) \). The second-order moments then saturate the uncertainty relation and their values are

\[
(\Delta \alpha)^2|_{t=0} = \frac{\hbar}{2}, \quad (\Delta p_u)^2|_{t=0} = \frac{\hbar}{2}, \quad \Delta (\alpha p_u)|_{t=0} = 0.
\]

For a concrete comparison we select a state that is initially peaked about \( \langle \hat{a} \rangle = \alpha_0 \) and \( \langle \hat{p}_u \rangle = 0 \), so that \( z = \alpha_0 \). In order for the state to be semiclassical, we need \( \alpha_0 \) to be ‘significantly larger’ than \( \sqrt{\hbar} \). We make a concrete choice \( \alpha_0 = 10\hbar \). In figure 1 we plot alongside each other the classical and two quantum-corrected trajectories of the system.
starting from the above initial values. The two corrected trajectories were calculated using two different methods: the kinematical coherent state of section 2.2 and effective equations truncated at order $\hbar$, equations (34)–(38) of section 2.3.

The two quantum trajectories agree very well for much of the evolution shown. In figure 2 we plot the quantum evolution of the second-order moments generated by $\hat{\alpha}$ and $\hat{p}_\alpha$. The horizontal line on the plot represents approximate threshold of the semiclassical approximation, the point where expectation values and square roots of second-order moments are no longer separated by an order of magnitude. From the middle plot in particular it is clear that the semiclassical approximation breaks down somewhere between $\beta_s = 2 \alpha_0$ and $\beta_s = 3 \alpha_0$ as $\Delta p_\alpha$ is no longer ‘much smaller’ than $\alpha_0$. Up until that point both methods for quantum evolution are in close agreement in describing not only the trajectory in the $\alpha - p_\alpha$ space but also the evolution of the second-order moments themselves. Since semiclassicity was used to obtain the truncated system of equations, there is no reason to expect it to be accurate beyond $\beta_s = 3 \alpha_0$.

The two methods agree excellently where the domains of their applicability overlap. Both methods have their own strengths and weaknesses. The weakness of the semiclassically
3.1. Long-term behavior of the state

Knowing the state exactly allows us to plot the magnitude of the wavefunction and make precise long-term predictions. From figure 3 we see that after $\beta_* \approx 10\alpha_0$ the state becomes highly truncated effective equations should by now stand out—in some systems semiclassicality eventually breaks down and moments of high order dominate. Direct evaluation on the states does not rely on this approximation and remains a valid method for computing the wavefunction at all times. The shortcomings of the latter technique are less obvious and are of practical nature. In order to apply the method, one needs, first of all, to decompose the initial state as a sum of the eigenstates of the Hamiltonian, which for an arbitrary state and a typical Hamiltonian can be complicated. During evolution, each of the eigenstates acquires a phase factor and they need to be re-summed to compute the wavefunction at a later time. For an arbitrary state, the sum may converge very slowly requiring one to sum over a very large number of eigenstates to obtain an accurate description of the wavefunction. Finally, for expectation values and moments of observables, further integrations must be done. In systems of several degrees of freedom, this will add considerably to computation times.

If one is to make robust predictions, a range of initially semiclassical states with a variety of initial values of moments should be considered—the procedure is very complicated to implement using state decomposition but amounts to nothing more than simply changing the initial conditions in the case of the effective equations. In the subsections that follow, we use the methods separately and exploit their individual strengths.

Figure 3. Square magnitude of the coherent state ‘Newton–Wigner wavefunction’ evolved for $0 < \beta_* < 15\alpha_0$. 
quantum, spread out over an entire orbit. Expectation values can no longer be interpreted as the most probable outcome of a measurement.

In figure 4 we look at the long-term behavior of the leading order quantum degrees of freedom. The magnitudes of $(\Delta \alpha)^2$ and $(\Delta p_\alpha)^2$ rise rapidly until around $\beta + \alpha_0 = 40$; thereafter, moments keep oscillating with a stable amplitude for as long as the evolution has been traced, up to around $\beta + \alpha_0 = 105$. As can be seen from the example of $\langle (\hat{\alpha} - \langle \hat{\alpha} \rangle)^3 \rangle$ in figure 4, third-order moments follow a similar pattern.

As expected, semiclassicality eventually breaks down and quantum fluctuations become large; this trend is illustrated by the evolving uncertainty measure $(\Delta \alpha)^2(\Delta p_\alpha)^2 - (\Delta(\alpha p_\alpha))^2$ (bounded below by the uncertainty relation) shown in figure 5. After the initial increase, there is a period of approximate stability; then the leading-order fluctuations start to oscillate with large amplitudes. Even though some moments return to small values during these oscillations, semiclassicality is not regained as shown by the long-term behavior of the uncertainties in figure 5. Details of this behavior, found numerically, appear rather characteristic, but it is difficult to find an explanation based on the underlying equations.

3.2. Short-term evolution with varying initial conditions

We now evolve effectively starting from the same initial expectation values, but varying the initial values of second-order moments. By the specific choices, some sets of moments used
Figure 5. Short-term (left) and long-term (right) coherent state evolution of the ‘quantum uncertainty’ defined as $(\Delta \alpha)^2(\Delta p_\alpha)^2 - (\Delta (\alpha p_\alpha))^2$ in units of $\hbar^2$.

Figure 6. Effective evolution of semiclassical states with different initial values of moments for $0 < \beta_\alpha < 3.5\alpha_0$. The initial values of moments are as follows. Dashed line—the original coherent state: $(\Delta \alpha)^2 = (\Delta p_\alpha)^2 = 0.005\alpha_0^2$, $\Delta (\alpha p_\alpha) = 0$. Dotted line: $(\Delta \alpha)^2 = 0.025\alpha_0^2$, $(\Delta p_\alpha)^2 = 0.001\alpha_0^2$, $\Delta (\alpha p_\alpha) = 0$. Thin solid line: $(\Delta \alpha)^2 = 0.001\alpha_0^2$, $(\Delta p_\alpha)^2 = 0.025\alpha_0^2$, $\Delta (\alpha p_\alpha) = 0$. Thick solid line: $(\Delta \alpha)^2 = 0.008\alpha_0^2$, $(\Delta p_\alpha)^2 = 0.008\alpha_0^2$, $\Delta (\alpha p_\alpha) = 0.005\alpha_0^2$.

here no longer saturate the uncertainty relations, and some have non-vanishing correlations. They cannot correspond to Gaussian states, and so their initial configurations would be much more difficult to implement using wavefunctions of physical states. The results are plotted in figure 6. In figure 7, we plot the corresponding effective evolution of moments for each set of the initial conditions, where the thin horizontal line approximately indicates the threshold of the semiclassical approximation for the second-order moments at $0.04\alpha_0^2$.

Larger $(\Delta \alpha)^2$ results in a larger deviation from the classical behavior and a faster breakdown of the semiclassical approximation. The above effect is much less sensitive to the momentum spread $(\Delta p_\alpha)^2$. This disparity between the effects of the two spreads may seem surprising given the symmetry between $\hat{\alpha}$ and $\hat{p}_\alpha$ in the expression for the physical Hamiltonian. This symmetry, however, is broken by the initial state we have chosen, which is peaked about $(\hat{p}_\alpha) = 0$ and $(\hat{\alpha}) = \alpha_0$, so that the spread in $\alpha$ produces a larger spread in the energy than the spread in $p_\alpha$. For all four corrected trajectories the bounce occurs at a larger value of $\alpha$ than the classical bounce.
4. Effective evolution of a radiation-filled universe

In this section we use the effective equations on their own to analyze quantum corrections to the dynamics of a radiation-filled Bianchi I universe briefly mentioned in section 2. This model has a more realistic matter content than the one analyzed above. We recall that the energy density of radiation has the form \( \rho \propto a^{-4} = e^{-4\alpha} \), which results in the Hamiltonian constraint \( C = p_\alpha^2 - e^{2\alpha} = 0 \). The constraint condition may be implemented effectively in a manner very similar to the way it was done in section 2.3; however, the physical inner product treatment would require a detailed knowledge of the (now continuous) spectrum of an operator that is completely different from \( \hat{H} \) that was used in (15) and is not straightforward to obtain. Even if we could determine energy eigenstates, expanding Gaussians or other general semiclassical states in this basis would be challenging. For this reason we do not attempt to implement the constraint of the radiation-filled model on the kinematical Hilbert space and restrict our analysis to the effective procedure, demonstrating its wide applicability.

4.1. Classical behavior

We deparametrize the constraint exactly as in section 2.1, selecting \( \beta_\alpha \) as time. The dynamics on \( \alpha \) and \( p_\alpha \) is then generated by the Hamiltonian \( H = \sqrt{p_\alpha^2 - e^{2\alpha} \nu} \) and results in the equations of motion \( d\alpha/d\beta_\alpha = p_\alpha/H \) and \( dp_\alpha/d\beta_\alpha = e^{2\alpha} \nu/H \). Noting that \( H \) is once again a constant of motion, we can immediately infer the classical phase-space trajectories, which are
of the form $p_\alpha = \pm \sqrt{e^{2\beta_+}} + \text{const}$. They split the $\alpha - p_\alpha$ space into three regions as illustrated in figure 8. There are no classical orbits in region 3, as $H$ becomes complex.

For the purpose of finding the dynamics driven by $H$ in terms of $\beta_+$ as time we can combine the two coupled first-order ordinary differential equations into a single second-order equation just as we have done for the model of section 2:

$$\frac{d^2\alpha}{d\beta_+^2} = \frac{1}{H} \frac{dp_\alpha}{d\beta_+} = \frac{1}{H^2} \sqrt{e^{2\beta_+}} e^{2\alpha}.$$  

This equation is not easy to integrate directly; it is more convenient to simplify it first. Recalling the explicit expression for $H$, we rewrite the right-hand side

$$\frac{d^2\alpha}{d\beta_+^2} = 1 - \frac{p_\alpha^2}{H^2},$$

which after substituting the equation of motion for $p_\alpha$ becomes

$$\frac{d^2\alpha}{d\beta_+^2} = 1 - \left( \frac{d\alpha}{d\beta_+} \right)^2.$$  

The explicit solution to this equation of motion is given by

$$\alpha(\beta_+) = \beta_+ - \log(1 + A e^{2\beta_+}) + B,$$  

where the integration constants $A$ and $B$ can be related to the initial values $\alpha_0 := \alpha(0)$ and $p_{\alpha 0} := p_\alpha(0)$ via

$$A = 1 + \frac{2p_{\alpha 0}}{e^{2\beta_+}} \sqrt{p_{\alpha 0}^2 - e^{2\beta_+}} - p_{\alpha 0},$$

$$B = \log \left( 2 + \frac{2p_{\alpha 0}}{e^{2\beta_+}} \sqrt{p_{\alpha 0}^2 - e^{2\beta_+}} - p_{\alpha 0} \right) + \alpha_0.$$  

Figure 8. Disjoint regions of classical solutions. Region 1: trajectories have the shape $p_\alpha = \sqrt{e^{2\beta_+}} + \text{const}$, and they correspond to expanding universes as $\alpha$ increases with $\beta_+$. Region 2: trajectories have the shape $p_\alpha = -\sqrt{e^{2\beta_+}} + \text{const}$, and they correspond to contracting universes as $\alpha$ decreases with $\beta_+$. Region 3: no classical solutions.
In terms of $A$ and $B$, the constant of motion is

$$H^2 = \frac{-e^{2B}v}{4A}.$$  

In order for $H$ to be real, we need $A < 0$, which, as one can check using the explicit expression above, holds everywhere in regions 1 and 2.\footnote{In fact $A \in (-1, 0)$ for the orbits in region 1 and $A \in (-\infty, -1)$ for the orbits in region 2. This means in particular that in region 2 the arguments of the logarithms in (39) and in the expression for $B$ are negative so that the values of the logarithms are complex. We point out that so long as the same convention for extending logarithm to the complex plane is used in both cases, the imaginary parts cancel each other out upon substitution of $B$ into (39) so that the value of $\alpha$ one obtains is real.} Using (39), $p_\alpha(\beta_\alpha)$ may be recovered from the equations of motion as $p_\alpha(\beta_\alpha) = H\dot{\alpha}/\ddot{\beta}_\alpha$.

For the orbits in region 1, $\alpha$ and $p_\alpha$ reach infinity at a finite positive value of the evolution parameter, namely at $\beta_\alpha = \alpha_0 - \log(p_{\alpha 0} - H)$. Explicit integration of expression (11) for the proper time using the above solution for $\alpha(\beta_\alpha)$ shows that this value of $\beta_\alpha$ is reached in infinite proper time. In other words, the expansion, as expected for the radiation-filled universe, takes infinite proper time, but anisotropy asymptotically approaches a maximum value. For the orbits in region 2 one can obtain a similar result by tracing evolution backward in time; in this case, $\alpha$ reaches infinity and $p_\alpha$ reaches negative infinity at $\beta_\alpha = \alpha_0 - \log(|p_{\alpha 0}| + H)$, which is always negative in that region.

Following those orbits forward in time, one finds that the collapse happens only as $\beta_\alpha$ goes to infinity. Once again one can use (11) to convert this to a proper time interval, with the result that evolution in $\beta_\alpha$ takes a finite amount of proper time:

$$\Delta \tau := \tau(\beta_\alpha = \infty) - \tau(\beta_\alpha = 0) = \frac{a_0^3 e^{2B}}{32\sqrt{|A|}v} \left( \frac{1 + |A|}{(|A| - 1)^2} - \coth^{-1} \left( \frac{\sqrt{|A|}}{|A|} \right) \right).$$

In this model, with positive energy, the singularity is certainly not resolved.

### 4.2. Effective constraints

Following the effective procedure for solving constraints outlined in section 2.3, we find the constraint functions truncated at second order:

$$C = (\hat{p}_\alpha)^2 - (\hat{p}_\alpha)^2 + e^{2o_\alpha}v + (\Delta p_\alpha)^2 - (\Delta p_\alpha)^2 + 2e^{2o_\alpha}v(\Delta \alpha)^2 = 0$$ (40)

$$C_{\beta_\alpha} = 2(\hat{p}_\alpha)\Delta(\beta_\alpha)\hat{p}_\alpha + i\hbar(\hat{p}_\alpha) - 2(\hat{p}_\alpha)\Delta(\beta_\alpha)\hat{p}_\alpha + 2e^{2o_\alpha}v(\Delta \beta_\alpha) = 0$$ (41)

$$C_{p_\alpha} = 2(\hat{p}_\alpha)(\Delta p_\alpha)^2 - 2(\hat{p}_\alpha)\Delta(\beta_\alpha)\hat{p}_\alpha + 2e^{2o_\alpha}v(\Delta \beta_\alpha) = 0$$ (42)

$$C_{\alpha} = 2(\hat{p}_\alpha)\Delta(\alpha)\hat{p}_\alpha - 2(\hat{p}_\alpha)\Delta(\alpha)\hat{p}_\alpha - i\hbar(\hat{p}_\alpha) + 2e^{2o_\alpha}v(\Delta \alpha)^2 = 0$$ (43)

$$C_{p_\alpha} = 2(\hat{p}_\alpha)(\Delta p_\alpha)^2 - 2(\hat{p}_\alpha)(\Delta p_\alpha)^2 + 2e^{2o_\alpha}v(\Delta \alpha p_\alpha) - i\hbar e^{2o_\alpha}v = 0.$$ (44)

These can be solved and gauge fixed following the same steps as for the model of section 2.3, with the result that evolution in $\beta_\alpha$ on the expectation values and moments of $\hat{\alpha}$ and $\hat{p}_\alpha$ is
generated by the quantum Hamiltonian

\[ H_Q = \sqrt{(\hat{p}_\alpha)^2 - e^{2(\hat{\beta})_\nu}} \left( 1 + e^{2(\hat{\beta})_\nu} - \frac{(\Delta p_\alpha)^2}{2((\hat{p}_\alpha)^2 - e^{2(\hat{\beta})_\nu})^2} + O((\Delta p_\alpha)^4) + O((\Delta \alpha)^4) + O((\Delta (\alpha p_\alpha))^2). \]  

(45)

The equations of motion are obtained by taking the quantum Poisson bracket between quantum variables and the quantum Hamiltonian:

\[ \frac{d(\hat{\beta}_\nu)}{d\beta_\nu} = \frac{\langle \hat{p}_\alpha \rangle}{\sqrt{(\hat{p}_\alpha)^2 - e^{2(\hat{\beta})_\nu}}} \]

\[ + e^{2(\hat{\beta})_\nu} \frac{\langle \hat{p}_\alpha \rangle \left( \langle \hat{p}_\alpha \rangle^2 + \frac{1}{4} e^{2(\hat{\beta})_\nu} (\Delta \alpha)^2 - \Delta (\alpha p_\alpha) (2 \langle \hat{p}_\alpha \rangle)^2 + e^{2(\hat{\beta})_\nu} + \frac{1}{2} \langle \hat{p}_\alpha \rangle (\Delta p_\alpha)^2 \right)}{2((\hat{p}_\alpha)^2 - e^{2(\hat{\beta})_\nu})^2}. \]

(46)

\[ \frac{d(\hat{p}_\alpha)}{d\beta_\nu} = \frac{\langle \hat{p}_\alpha \rangle}{\sqrt{(\hat{p}_\alpha)^2 - e^{2(\hat{\beta})_\nu}}} \]

\[ + e^{2(\hat{\beta})_\nu} \left( \langle \hat{p}_\alpha \rangle \left( (\hat{p}_\alpha)^2 + \frac{1}{2} e^{2(\hat{\beta})_\nu} - 2 (\Delta (\alpha p_\alpha))^2 (\Delta \alpha)^2 - 2 \Delta (\alpha p_\alpha) \left( \frac{1}{2} e^{2(\hat{\beta})_\nu} + \langle \hat{p}_\alpha \rangle^2 \right) \right) \right) \]

\[ + e^{2(\hat{\beta})_\nu} \frac{(\Delta p_\alpha)^2}{2((\hat{p}_\alpha)^2 - e^{2(\hat{\beta})_\nu})^2} \]

\[ + e^{2(\hat{\beta})_\nu} \frac{(\Delta (\alpha p_\alpha))^2}{2((\hat{p}_\alpha)^2 - e^{2(\hat{\beta})_\nu})^2} \]

\[ + e^{2(\hat{\beta})_\nu} \frac{(\Delta (\alpha p_\alpha))^2}{2((\hat{p}_\alpha)^2 - e^{2(\hat{\beta})_\nu})^2}. \]

(47)

As before, these equations reduce to the classical equations of motion at zeroth order in moments and are straightforward to evolve numerically.

4.3. Numerical evolution

In this section we take a classical phase space trajectory from each of the regions 1 and 2 and compare the effective trajectories for a variety of semiclassical states initially peaked about these classical solutions. Effective and classical trajectories of the expanding universe are plotted in figure 9. Clearly, the significance of quantum back-reaction can be seen well before the approximation breaks down.

\[ \frac{d(\Delta \alpha)^2}{d\beta_\nu} = \frac{2 e^{2(\hat{\beta})_\nu} ((\hat{p}_\alpha)^2 - (\Delta \alpha)^2)}{((\hat{p}_\alpha)^2 - e^{2(\hat{\beta})_\nu})^2} . \]

(48)

\[ \frac{d(\Delta p_\alpha)^2}{d\beta_\nu} = \frac{2 e^{2(\hat{\beta})_\nu} (2 \langle \hat{p}_\alpha \rangle^2 - e^{2(\hat{\beta})_\nu} (\Delta \alpha)^2 - (\hat{p}_\alpha) (\Delta p_\alpha)^2)}{((\hat{p}_\alpha)^2 - e^{2(\hat{\beta})_\nu})^2} . \]

(49)

\[ \frac{d(\Delta (\alpha p_\alpha))^2}{d\beta_\nu} = \frac{e^{2(\hat{\beta})_\nu} (2 \langle \hat{p}_\alpha \rangle^2 - e^{2(\hat{\beta})_\nu} (\Delta \alpha)^2 - (\Delta p_\alpha)^2)}{((\hat{p}_\alpha)^2 - e^{2(\hat{\beta})_\nu})^2} . \]

(50)

For semiclassical states, restrictions on (\hat{\beta}) and (\hat{p}_\alpha) follow from this Hamiltonian since those states cannot tunnel arbitrarily deeply into the classically forbidden region. The part of the quantum phase space parametrized by (\hat{\beta}) and (\hat{p}_\alpha) is thus not of the form \( \mathbb{R}^2 \), and a quantization of the reduced phase space would require more complicated representations of the basis operators. In our method, we need to assume well-defined representations only of the kinematical operators for which no restrictions arise. After solving the constraints, we do obtain physical expectation values and fluctuations corresponding to a quantization of the reduced phase space, but our method does not require us to make assumptions about physical operators. In this way, the usual difficulties in constructing physical Hilbert space representations are sidestepped.
Figure 9. Phase space trajectories of an expanding universe classical (dotted) and effective with different initial values for second-order moments: dashed line—\((\Delta \alpha)^2 \nu = 0.001H_0^2\), \((\Delta p_\alpha)^2 = 0.025H_0^2\), \(\Delta (p_\alpha)\sqrt{\nu} = 0\); thin solid line—\((\Delta \alpha)^2 \nu = 0.025H_0^2\), \((\Delta p_\alpha)^2 = 0.001H_0^2\), \(\Delta (p_\alpha)\sqrt{\nu} = 0\); thick solid line—\((\Delta \alpha)^2 \nu = 0.008H_0^2\), \((\Delta p_\alpha)^2 = 0.008H_0^2\), \(\Delta (p_\alpha)\sqrt{\nu} = 0.005H_0^2\). Solutions were evolved for \(0 < \beta_s < 0.2\); the vertical line indicates the breakdown of the semiclassical approximation based on the size of second-order moments.

Figure 10. Evolution of second-order moments in an expanding universe. \((\Delta \alpha)^2 \nu\) (dashed), \((\Delta p_\alpha)^2\) (solid), \(\Delta (p_\alpha)\sqrt{\nu}\) (dotted), with initial values: left—\((\Delta \alpha)^2 \nu = 0.008H_0^2\), \((\Delta p_\alpha)^2 = 0.008H_0^2\), \(\Delta (p_\alpha)\sqrt{\nu} = 0.005H_0^2\); middle—\((\Delta \alpha)^2 \nu = 0.025H_0^2\), \((\Delta p_\alpha)^2 = 0.001H_0^2\), \(\Delta (p_\alpha)\sqrt{\nu} = 0\); right—\((\Delta \alpha)^2 \nu = 0.001H_0^2\), \((\Delta p_\alpha)^2 = 0.025H_0^2\), \(\Delta (p_\alpha)\sqrt{\nu} = 0\).

The corresponding evolution of the leading order moments starting from different initial values is plotted in figure 10, where the horizontal line, as before, indicates an approximate threshold of the semiclassical approximation for the second-order moments.

Effective and classical trajectories of the contracting universe are plotted in figure 11. The corresponding evolution of the leading-order moments starting from different initial values is
Figure 11. Phase space trajectories of a contracting universe classical (thin solid line) and effective with different initial values for second-order moments: dashed line—$(\Delta \alpha)^2 \nu = 0.001 H_0^2$, $(\Delta p_\alpha)\sqrt{\nu} = 0$; dotted line—$(\Delta \alpha)^2 \nu = 0.025 H_0^2$, $(\Delta p_\alpha)^2 = 0.001 H_0^2$, $\Delta (\alpha p_\alpha)\sqrt{\nu} = 0$; thick solid line—$(\Delta \alpha)^2 \nu = 0.025 H_0^2$, $(\Delta p_\alpha)^2 = 0.001 H_0^2$, $\Delta (\alpha p_\alpha)\sqrt{\nu} = 0.005 H_0^2$. Solutions were evolved for $0 < \beta^+ < 0.07$; the vertical line indicates the breakdown of the semiclassical approximation (coming from the right along the $\alpha$-axis).

plotted in figure 12, where the horizontal line, once again, indicates an approximate threshold of the semiclassical approximation for the second-order moments. Even in the absence of specific forms of physical semiclassical states in a Hilbert space representation, as was realized for our first model, the quantum dynamics can be analyzed self-consistently based on effective equations. Although the numerical solutions shown do not comprehensively cover the initial parameter space of our system they still warrant several observations. Specifically, we see that in general quantum back-reaction does have a noticeable effect on the phase-space trajectory of the system. Qualitatively, the back-reaction speeds up anisotropy growth with respect to
the scale factor for the expanding universe and slows it down for the contracting universe. This can be inferred indirectly, by noting that for each trajectory in figure 9, $\beta_+$ grows from 0 to 0.2, at which point the scale factors are larger for the quantum corrected trajectories. Similarly for each trajectory in figure 11, $\beta_+$ evolves from 0 to 0.07, where quantum-corrected trajectories reach a smaller scale factor than the classical one. The magnitude of the effect that the back-reaction has does depend on the specifics of the quantum state.

5. Conclusions

Most quantum systems of physical relevance can only be analyzed by perturbation methods. Quantum gravity and quantum cosmology cannot be considered exceptions. As demonstrated by the examples of this paper, canonical effective equations, based on the back-reaction of moments of a state on its expectation values, are of wide applicability, capture quantum effects reliably and approximate the full quantum dynamics in a self-consistent way. They are tractable even in situations in which semiclassical wavefunctions in physical Hilbert spaces would be too complicated to be constructed—cases that abound in quantum cosmology and quantum gravity.

Acknowledgments

This work was supported in part by NSF grant PHY 0748336.

References

[1] Cametti F, Jona-Lasinio G, Presilla C and Toninelli F 2000 Comparison between quantum and classical dynamics in the effective action formalism *Proc. Int. School of Physics ‘Enrico Fermi’, Course CXLIII* (Amsterdam: IOS Press) pp 431–48 (arXiv:quant-ph/9910065)
[2] Bojowald M and Skirzewski A 2006 Effective equations of motion for quantum systems Rev. Math. Phys. 18 713–45
[3] Bojowald M 2007 Large scale effective theory for cosmological bounces *Phys. Rev. D* 75 081301
[4] Bojowald M 2007 Dynamical coherent states and physical solutions of quantum cosmological bounces *Phys. Rev. D* 75 123512
[5] Bojowald M 2008 Quantum nature of cosmological bounces *Gen. Rel. Grav.* 40 2659–83
[6] Bojowald M, Sandhöfer B, Skirzewski A and Tsobanjan A 2009 Effective constraints for quantum systems *Rev. Math. Phys.* 21 111–54
[7] Bojowald M and Tsobanjan A 2009 Effective constraints for relativistic quantum systems Phys. Rev. D 80 125008
[8] Misner C W 1969 Mixmaster universe Phys. Rev. Lett. 22 1071–4
[9] Hartle J B and Marolf D 1997 Comparing formulations of generalized quantum mechanics for reparametrization-invariant systems Phys. Rev. D 56 6247–57
[10] Haag R 1992 Local Quantum Physics (Berlin: Springer)
[11] Newton T D and Wigner E P 1949 Localized states for elementary systems Rev. Mod. Phys. 21 400–6
[12] Barnich G and Grigoriev M 2005 Hamiltonian BRST and Batalin–Vilkovisky formalisms for second quantization of gauge theories Commun. Math. Phys. 254 581–601