Feasibility of a Unitary Quantum Dynamics in the Gowdy $T^3$ Cosmological Model

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It has been pointed out that it is impossible to obtain a unitary implementation of the dynamics for the polarized Gowdy $T^3$ cosmologies in an otherwise satisfactory, nonperturbative canonical quantization proposed for these spacetimes. By introducing suitable techniques to deal with deparametrized models in cosmology that possess an explicit time dependence (as it is the case for the toroidal Gowdy model), we present in this paper a detailed analysis about the roots of this failure of unitarity. We investigate the impediments to a unitary implementation of the evolution by considering modifications to the dynamics. These modifications may be regarded as perturbations. We show in a precise manner why and where unitary implementability fails in our system, and prove that the obstructions are extremely sensitive to modifications in the Hamiltonian that dictates the time evolution of the symmetry-reduced model. We are able to characterize to a certain extent how far the model is from unitarity. Moreover, we demonstrate that the dynamics can actually be approximated as much as one wants by means of unitary transformations.

PACS numbers: 04.60.Ds, 04.62.+v, 04.60.Kz, 98.80.Jk

I. INTRODUCTION

Symmetry-reduced models have been used over the past 30 years as an appropriate arena to test strategies aimed for the quantization of the full theory of gravity within the canonical approach, as well as toy models which can provide us with insights about the kind of phenomena that should be expected in quantum general relativity. Most of the examples of symmetry-reduced models studied so far are minisuperspace models [1], namely, simple systems where the reduction leaves only a finite number of physical degrees of freedom. There is another class of models which has more interest inasmuch as they retain the field complexity of general relativity. These are the so-called midisuperspace models (for a recent review see Ref. [2]), which after reduction possess an infinite number of degrees of freedom. Thus, their quantization would lead to a true quantum field theory.

Within this class, and together with the Einstein-Rosen waves [3], the model that has deserved more attention lately is the Gowdy $T^3$ cosmological model [4, 5, 6, 7, 8]. This model was introduced by Gowdy during the seventies in a systematic search for all spacetimes with two commuting spacelike Killing vector fields and compact spatial hypersurfaces [10]. Apart from the $T^3$ topology of a three-torus, the other two possible spatial topologies for the Gowdy spacetimes are the three-handle $S^1 \times S^2$ and the three-sphere $S^3$ (or the topology of a manifold covered by one of the above). The interest in the Gowdy $T^3$ model can thus be easily understood, since it provides the simplest of all the inhomogeneous, empty, spatially closed cosmological systems. The genuine field-theory character of this model and its possible applications in cosmology make it a natural candidate to study fundamental questions about canonical quantum gravity and quantum field theory in curved spacetimes.

Its quantization was already considered in the seventies [11], and revisited both in the eighties [12, 13, 14] and more recently [4, 5, 6, 7, 8]. The first preliminary attempts to define a quantum theory and extract physics from the Gowdy $T^3$ model [11, 12] were followed by more detailed analysis [4, 5] that discussed the nonperturbative quantization of the system employing the Ashtekar formulation of Lorentzian general relativity [13]. Considerable progress has been achieved lately in defining a complete quantization of the (sub-)model with linear polarization, in which both Killing vectors are hypersurface orthogonal [5]. The proposed quantization is based on the fact that the polarized model can be equivalently treated as $2 + 1$ gravity coupled to a massless scalar field, defined on a manifold whose topology is $T^2 \times \mathbb{R}$.

One important aspect in the study of quantum cosmological models is their dynamical evolution. For the polarized Gowdy $T^3$ model with the particular quantization performed in Ref. [5], it has been recently shown that the dynamics is not implementable at the quantum level as a unitary transformation [4, 7]. From the point of view of canonical quantum gravity, this result does not represent a serious drawback for the simple reason that (owing to the compact nature of the spatial slices) time evolution is pure gauge in the Hamiltonian description. Hence, there is no time evolution and no dynamics. The system is endowed with a fictitious dynamics via a “deparametrization” procedure, and there is no apparent reason to select a preferred deparametrization.

Nevertheless, if one accepts that unitary evolution is a key ingredient in conventional (field) quantum theory, necessary in order to pose physically meaningful questions for issues like those concerning the initial singularity in cosmology, the lack of a unitary time evolution is a drawback for the kind of quantization put forward in Ref. [5]. From that quantum theory, one would not be able to extract predictions for different instants of time, because probability is not conserved. In this sense, the quantization is not fully consistent [4]. Thus, restoration of unitarity in the evolution seems a fundamental

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issue in order to achieve a satisfactory quantization of the polarized Gowdy $T^3$ model. A rigorous quantization along these lines will provide us with a specific example of midisuperspace that can be very helpful, as a point of reference for comparisons, for a future quantization starting from loop quantum gravity (where impressive progress has been made, but exclusively for minisuperspaces [16]) or for implementations of the “consistent discretization” approach [17] (which has recently been applied to the Gowdy model [18]).

In this work, we will explore the reasons behind the failure in the unitary implementability of the dynamics as a first step in proposing solutions to it or introducing alternative descriptions for the quantum evolution. Although the lack of unitarity certainly follows from the absence of square summability for the antilinear part of the Bogoliubov transformation which relates the annihilation (creation) operator at, say, the “final” time $t_f$ with the annihilation and creation operators at an “initial” time $t_i$ [6][7], we want to analyze in detail the roots of this failure. We will show in a precise manner why unitary implementability fails in our system and, in a certain sense, we will be able to characterize how far the model is from unitarity. In doing so, we will introduce suitable techniques to deal with deparametrized models in cosmology that possess an explicit time dependence, like the Gowdy one.

The structure of the paper is as follows. In Sec. II we obtain the reduced phase space of the system by performing the symmetry reduction and introducing a deparametrization procedure in order to (partially) fix the gauge freedom and select a Hamiltonian vector field to represent the dynamics. This reduction and gauge-fixing process had not been presented before starting with the spacetime metric of the model in general relativity, although the resulting description of the vacuum Gowdy spacetimes is essentially the same that was discussed in Refs. 5[6] (except for the remark on footnote1) and Ref. 7. Therefore, the quantum theory on which we will base our analysis is that constructed by Pierri 5 (or, equivalently, that analyzed in Ref. 7).

Sec. III is divided in three parts. In the first one, we review the dynamics of the scalar field that represents (most of) the vacuum radiation, as a point of reference for comparisons. In this part, a crucial remark is that the coordinates of the covariant phase space (namely the coefficients that determine the field in terms of an orthonormal basis of solutions -defined essentially by the negative of the complex structure given in Ref. 5-) do not evolve in time. In these coordinates, the generator of the evolution is obviously the zero Hamiltonian. The dynamics will be introduced through a time-dependent map from the covariant to the canonical phase space. In the remaining parts of the section, we will investigate the impediments for a unitary implementation of the evolution by considering modifications to the dynamics that may be regarded as small perturbations. We will be able to identify where the failure of unitarity comes from and, in the last subsection, prove that the severity of the problem is greatly ameliorated by the fact that small corrections to the dynamics can be implemented in a unitary way. In addition, our analysis makes clear that the diagonalization of the Hamiltonian performed in Ref. 6[8] is just an instantaneous diagonalization which ignores the change in time of the Bogoliubov coefficients. Here, these time variations are explicit and rigorously taken into account. Finally, the conclusions and some further comments are presented in Sec. IV.

One appendix is added which contains a proof about the behavior of the coefficients employed in the main discussion. In the following, lower case Latin indices on a tensor will denote its purely spatial components, whereas capital case Latin indices will be used to denote the tensor itself (abstract index notation).

II. THE POLARIZED GOWDY MODEL

The polarized Gowdy $T^3$ model describes globally hyperbolic four-dimensional vacuum spacetimes, $(\mathcal{M}, g_{AB})$, with two commuting hypersurface orthogonal spacelike Killing fields and compact spacelike hypersurfaces homeomorphic to a three-torus. Since global hyperbolicity implies that we can foliate $(\mathcal{M}, g_{AB})$ by Cauchy surfaces, $\Sigma$, parametrized by a global time function $t$, then a $3+1$ decomposition is available and the line element can be written

$$ds^2 = -N^2 dt^2 + h_{ij}(dx^i + N^i dt)(dx^j + N^j dt), \quad (1)$$

where we choose $t \in \mathbb{R}^+$, the coordinates in the sections of constant time are $\{x^i\} := \{x^1 = \theta, x^2 = \sigma, x^3 = \delta\}$ with $x^i \in S^1$, $N$ and $\{N^i\}$ are, respectively, the lapse function and the components of the shift vector $N^i$, and $\{h_{ij}\}$ are the components of the induced spatial metric $h_{AB}$.

In addition, we will impose that $\partial / \partial x^a \cdot a = 2, 3$ are the two spacelike Killing vector fields. Thus, the metric must be independent of the coordinates $x^a$. Moreover, performing a (partial) gauge fixing along the lines explained in Ref. 13 (for pure gravitational plane waves) and Ref. 20 (for cylindrical spacetimes), remembering that the metric functions must be periodic in $\theta$, and using that $\partial / \partial x^a \cdot a$ are commuting hypersurface orthogonal vector fields, one gets a line element for the reduced model of the form

$$ds^2 = -N^2 dt^2 + h_{\theta \theta}[d\theta + N^\theta dt]^2 + \sum_{a=2}^3 h_{aa}(dx^a)^2. \quad (2)$$

Let us consider now the following change of metric variables $\{h_{ij}\} \mapsto \{Q^a\} := \{\psi, \gamma, \tau\}$, defined by

$$h_{\theta \theta} = e^{\tau - \psi}, \quad h_{\sigma \sigma} = e^{\phi - \tau^2}, \quad h_{\delta \delta} = e^{\phi}. \quad (3)$$

Since this change is just a point transformation, the momenta $P_a$ canonically conjugate to $Q^a$ are

$$P_a = p_{ij} \frac{\partial h_{ij}}{\partial Q^a}. \quad (4)$$

1 The “q-number” nature of the time variable which occurs in Refs. 6[8] will be avoided here by introducing a gauge condition that is slightly different to the one imposed in those references; in this way the physical degrees of freedom will be neatly disentangled from the time variable. This type of mixing is also absent in Ref. 7; however, the disentanglement is attained there thanks to the introduction of an appropriate (partially) reduced line element since the very beginning, rather than to its construction by gauge fixing.
where $p^{ij} = \sqrt{h}(K^{ij} - Kh^{ij})$ are the momenta canonically conjugate to $h_{ij}$, we have set the Newton constant $G$ equal to $\pi/4$, $h$ is the determinant of the induced metric, and $[K^{ij}]$ are the components of its extrinsic curvature, with trace equal to $K$. Substituting in Eq. (2) our new set of variables and introducing the densitized lapse factor $N := N/\sqrt{h}$, we arrive at the line element

$$ds^2 = e^\theta(-\tau^2N^2dt^2 + [d\theta + N^\theta dt]^2)$$

$$+ e^\phi(\tau^2d\sigma^2 + e^{2\phi}d\delta^2),$$

(5)

whose Einstein-Hilbert action is then given by

$$S = \int_h^{\Omega} dt \int d\theta \left[ P_\tau Q^\theta - \mathcal{H}(Q^\theta, P_\theta) \right]$$

$$= \int_h^{\Omega} dt \int d\theta \left[ P_\tau \dot{\tau} + P_\gamma \dot{\gamma} + P_\phi \dot{\phi} - (N\dot{C} + N^\theta C_0) \right].$$

(6)

The presence of the remaining first class constraints $\tilde{C}$ and $C_0$ reflects the fact that the gauge has been only partially fixed. These (densitized) Hamiltonian constraint and momentum constraint are, respectively,

$$\tilde{C} := \frac{1}{2}(P_\phi^2 - 2\tau P_\phi \tau_\phi) - \frac{1}{2}(4\tau'' - 2\gamma' + \tau\phi'^2),$$

$$C_0 := P_\tau \tau' + P_\gamma \gamma' + P_\phi \phi' - 2P_\phi^\prime.$$

(7)

The prime denotes the derivative with respect to $\theta$.

Note that, since the spatial slices are compact, there exist no boundary contributions to the Hamiltonian. Therefore, the total Hamiltonian vanishes on the constraint surface and there is no distinction between gauge and dynamics. It is then necessary to carry out a deparametrization in order to introduce dynamics. This deparametrization is accomplished as part of a gauge fixing of the model: one imposes suitable conditions which, together with the constraints (7), form a set of second class constraints, allowing the reduction of the system. Explicitly, we demand the following gauge fixing conditions (which are a slight modification of those introduced in Refs. 4, 5)

$$g_1 := P_\phi + p = 0, \quad g_2 := \tau - tp = 0.$$  

(8)

The first of these conditions requires the momentum canonically conjugate to $\tau$ to be homogeneous (independent of $\theta$). Furthermore, this homogeneous part is a constant (of motion) $p$. In this sense, it is worth pointing out that the Poisson brackets of $\hat{f}P_\phi/(2\pi)$ (i.e. $-p$) with all the first class constraints (7) vanish weakly, so that it is indeed a Dirac observable. On the other hand, the second of our conditions fixes the metric function $\tau$ equal to the global time function $t$ except for a rescaling that is constant on shell, though can vary on different solutions. Modulo constraints and gauge-fixing conditions, a straightforward calculation shows then that

$$\{g_1, \int d\theta GC_0\} = -pG', \quad \{g_2, \int d\theta FC\} = tp^2F,$$

(9)

where the smearing functions $F$ and $G$ on $S^1$ are, respectively, a density of weight $-1$ and a scalar. Therefore, if $F$ and $G'$ are different from zero, these Poisson brackets do not vanish provided that $p \neq 0$. Thus, we have to restrict all considerations to the sector of solutions with nonzero $p$ in order to get a well-posed fixation.

The next step in this procedure consists in demanding the compatibility of the gauge-fixing conditions with dynamics: the total time derivative of $g_1$ and $g_2$ must vanish for some choice of $N$ and $N^\theta$. This derivative is the sum of the Poisson bracket with the total Hamiltonian $\mathcal{H}$ and the partial derivative with respect to the explicit $t$-dependence. Modulo constraints and gauge-fixing conditions, we have

$$\dot{g}_1 = -p(N^\theta)' = \dot{N}_p, \quad \dot{g}_2 = -p + tp^2N.$$  

(10)

The requirements $\dot{g}_1 = 0$ and $\dot{g}_2 = 0$ are then satisfied if $N^\theta$ is any function of $t$ and $N = (tp)^{-1}$. It is worth noticing that, while the densitized lapse function is completely determined in this process, the shift function is not fully fixed. There remains some diffeomorphism gauge freedom, generated by the homogenous part of the constraint $C_0$ (after reduction). Besides, note that we have to further restrict $p$ to be positive in order to ensure the positivity of the lapse function $\tilde{N}$.

In order to extract the true degrees of freedom, one solves the set of second class constraints $\{C_0, g_1, g_2\}$, obtaining

$$pP_\tau = -\frac{1}{2}(P_\phi^2 + tp\phi'^2),$$  

(11)

$$py' = P_\phi \phi' := \Lambda.$$

(12)

By performing a Fourier expansion in $\theta$ of the functions $\gamma$ and $\Lambda$ (which is possible given the smoothness of the fields on $S^1$), it is not difficult to see that identity (12) allows us to solve for all modes of $\gamma$ but the zero mode. More precisely, the Fourier coefficients $\gamma_n$ are determined in terms of $\Lambda_n$ by $ip\gamma_n = \Lambda_n$. Thus, there is still an undetermined coefficient, namely $\gamma_0$, and consequently we are left with a global degree of freedom.

Furthermore, note that integration over $S^1$ of Eq. (12) leads to the global constraint

$$\Lambda_0 = \frac{1}{\sqrt{2\pi}} \int d\theta P_\phi \phi' = 0,$$

(13)

which is essentially the homogenous part of the constraint $C_0$. Therefore, the diffeomorphism gauge freedom has not been entirely removed and the $\theta$-component of the shift vector cannot be completely fixed. However, as we have already seen, the only allowed dependence of $N^\theta$ is on $t$. This type of shift can always be absorbed by redefining our angular coordinate $\theta$ [4]. After our gauge fixing and the absorption of the
shift, the metric becomes
\[ ds^2 = e^{2\phi} (-dt^2 + d\theta^2) + e^{\phi} t^2 p^2 d\sigma^2 + e^{\phi} d\gamma^2 , \] (14)
\[ \gamma = \frac{q}{2\pi} - i \sum_{n \neq 0} \frac{\Lambda_n}{np} \frac{e^{int}}{\sqrt{2\pi}} , \] (15)
where \( q := \sqrt{2\pi} \gamma \) is the coordinate canonically conjugate to \(-p\) (the zero mode of \( P_\gamma / \sqrt{2\pi} \)).

The reduced action for the system (modulo a spurious boundary term \(-pq\) is)
\[ S_r = \int_{\Gamma_{t_{f}}}^{\Gamma_{t_{i}}} dt \left\{ \tilde{P}(q + \oint d\theta P) + \oint d\theta \left[ P_\phi \psi + pP_\tau \right] \right\} = \int_{\Gamma_{t_{f}}}^{\Gamma_{t_{i}}} dt \left\{ \eta q + \oint d\theta \left[ P_\phi \psi - \frac{1}{2} \left( \frac{P_\phi^2}{tp} + t p\psi' \right)^2 \right] \right\} , \]
\[ \eta := q - \oint d\theta \frac{1}{2p} \left( \frac{P_\phi^2}{tp} + t p\psi' \right)^2 . \] (16)

In the first equality, \( P_\tau \) denotes the solution given in Eq. (13). Thus, \( S_r \) is a functional on the reduced phase space \( \Gamma_r \), which is coordinatized by \((\eta, P_\phi, \psi, P_\psi)\), and where the (only nonvanishing) basic Poisson brackets are \([p, \eta] = 1\) and \([\psi(t, \theta), P_\phi(\theta, \bar{\theta})] = \delta(\theta - \bar{\theta}) \). Note that, owing to the presence of the global constraint (13), the space of physical states does not correspond to \( \Gamma_r \) but to a submanifold of it. However, since this submanifold is nonlinear, the reduction by the constraint is usually postponed to the quantum theory, where it is imposed as an operator condition on quantum states.

Let us now perform the canonical transformation
\[ \phi = \sqrt{t} \psi , \quad P_\psi = P_\phi \sqrt{t} , \]
\[ Q = -\eta + \frac{1}{2p} \oint d\theta P_\phi \psi , \]
\[ P = p . \] (17)

In terms of this new set of phase space variables the reduced action reads
\[ S_r = \int_{\Gamma_{t_{f}}}^{\Gamma_{t_{i}}} dt \left\{ \tilde{P} \tilde{Q} + \oint d\theta \left[ P_\phi \phi - \mathcal{H}_r \right] \right\} = \int_{\Gamma_{t_{f}}}^{\Gamma_{t_{i}}} dt \left\{ \mathcal{H}_r \right\} , \] (18)
where the (reduced) Hamiltonian density is
\[ \mathcal{H}_r = \frac{1}{2} \left( \frac{P_\phi^2}{t} + t p\phi' \right)^2 . \] (19)

Thus, our midisuperspace model consists of a phase space \( \tilde{\Gamma}_r \) coordinatized by the canonical pairs \((Q, P)\) and \((\phi, P_\phi)\), which we will call the global and local degrees of freedom, respectively. Remember that \( P \) is strictly positive. To arrive at a true canonical pair of real variables, we could always replace \((Q, P)\) with \((Q\bar{P}, \ln P)\). There also remains a global constraint on the system \((\Lambda_0 = 0)\) which restricts the physical states to lie in a submanifold of \( \tilde{\Gamma}_r \). Note that, given the \((Q, P)\)-independence of the Hamiltonian density, these “point particle” degrees of freedom are constants of motion. Hence a nontrivial evolution may only take place in the field sector \( \Gamma = \{ (\phi, P_\phi) \} \). Since the time evolution affects only the local degrees of freedom, we will focus on them in our analysis.

Varying action (18) with respect to \( \phi \) and \( P_\phi \) one gets the field equations
\[ P_\phi = t \phi , \quad P_\phi = t \phi'' . \] (20)

Hence, we only have to consider all smooth solutions to the second-order differential equation
\[ \phi + \frac{1}{t} \phi - \phi'' = 0 \] (21)
in order to specify the classical spacetime metric. Using the method of separation of variables, it is not difficult to see that these solutions, that we will generically denote by \( \varphi \), adopt the form
\[ \varphi(t, \theta) = \frac{1}{\sqrt{2\pi}} \sum_{n \in \mathbb{Z}, n \neq 0} \left[ A_n H_0(|n| t)e^{int} + A_n^* H_0(|n| t)e^{-int} \right] \]
\[ + \frac{1}{\sqrt{2\pi}} \left( \bar{q}_0 + \bar{p}_0 \ln t \right) , \] (22)
where the symbol \( \ast \) denotes complex conjugation, \( \bar{q}_0 \) and \( \bar{p}_0 \) are constants, \( H_0 \) is the zeroth-order Hankel function of the second kind \([21]\) and, in order to guarantee pointwise convergence, the sequence of constant coefficients \( \{ A_n \} \) has to decrease faster than the inverse of any polynomial in \( n \) as \( n \to \pm \infty \). Expression (22) determines the metric (14) (with \( \psi = \varphi / \sqrt{t} \)) except for the values of \((q, p)\). One can show that its Kretchmann scalar blows up at \( t = 0 \), so that there is an initial singularity and the global time function \( t \) must be strictly positive.

In the field sector, the physical phase space can be alternatively described by the submanifold obtained by imposing the constraint \( \Lambda_0 \) in \( \Gamma \), or by that submanifold of the space \( V \) of the smooth solutions \( \{ \varphi \} \) defined by the constraint
\[ \Lambda_0 := \sum_{n \in \mathbb{Z}, n \neq 0} n A_n^* A_n = 0 . \] (23)

In addition notice that, for the field sector, the reduced action (18) can be viewed as that corresponding to an axi-symmetric, massless, free scalar field propagating in the fictitious flat background in three dimensions:
\[ (f) g_{AB} = -(dt)A(dt)B + (d\theta)A(d\theta)B + \bar{r}^2 (d\sigma)A(d\sigma)B . \] (24)

Thus, we can identify \( \Gamma \) with the canonical phase space of the scalar field in this background, \((M \simeq T^3 \times \mathbb{R}^+, (f) g_{AB})\), whereas the space \( V \) of smooth solutions can be considered as the covariant phase space of such a Klein-Gordon field. Namely, \( \phi \) and \( P_\phi \) are the configuration and momenta on the constant-time section \( \Sigma_\tau \) of the scalar field \( \varphi \) propagating in \((M, (f) g_{AB})\). Besides, since the fictitious background is globally hyperbolic, given a smooth Cauchy surface \( \Sigma_0 \), there will be a natural isomorphism \( \{ \Sigma_\tau \} \) between the linear spaces \( \Gamma \) and \( V \). In this framework, the analysis of the dynamics of the polarized Gowdy \( T^3 \) model becomes equivalent to the study of the time evolution of the free scalar field. In the next section we review this dynamics and discuss the obstructions to its unitary quantum implementation.
III. DYNAMICS

It has recently been shown that the dynamical evolution generated by the reduced Hamiltonian $H_r = \not\!\not\!\not\!\not\!\not\not\!\not\not\not\!\not\not\not H_l$ [see Eq. (19)] cannot be implemented as a unitary transformation, neither on the kinematical Fock space $\mathcal{F}$ constructed from $V$ with the complex structure associated with the field decomposition $\Sigma$, nor in the physical Hilbert space of states $\mathcal{H}$ determined by the kernel of the operator version of the constraint $\Sigma$. We want to analyze in detail the reasons behind this lack of a unitary implementation and discuss how severe the problem is, studying whether small corrections (coming e.g. from quantum or perturbative modifications) to the dynamics may suffice to restore the unitarity.

For the space $V$, we will employ as coordinates the constants coefficients of the field decomposition $\Sigma$, whereas for $\Gamma$ we will use a different set that absorbs in its (implicit) time dependence all the evolution of the field. We will see that the dynamics in $\Gamma$ is dictated by $H_r$, whereas that in $V$ is frozen, because the considered coefficients are constants of motion 3.

For the sake of completeness and clarity, let us remember some definitions and make a few remarks that will be useful in our analysis. Firstly, we recall that given two field decompositions in different orthonormal bases of solutions, namely $\varphi = \sum_{n} A_n \phi_n(t, \theta) + \tilde{A}_n \phi'_n(t, \theta)$ and $\varphi = \sum_{n} \tilde{A}_n \phi_n(t, \theta) + \tilde{A}_n \phi'_n(t, \theta)$, their coefficients are related by a Bogoliubov transformation. That is, $\tilde{A}_n = \sum_{m} \alpha_{mn} A_m + \beta_{mn} \tilde{A}_m$ with $\sum_{m} (\alpha_{nm} \alpha_{mj} - \beta_{nm} \beta_{mj}^*) = \delta_{ij}$ and $\sum_{k} (\alpha_{ik} \beta_{jk} - \beta_{ik} \alpha_{jk}) = 0$ 22.

Secondly, as in the classical case, the quantum theory for the scalar field can be formulated either in a covariant or in a canonical approach. In fact, it is generally known that, by endowing the space of (smooth) solutions $V = \{\varphi\}$ to the Klein-Gordon equation with a complex structure $J$ compatible with the symplectic structure, one can construct in a canonical way the Hilbert space of the quantum theory as a symmetric Fock space $\mathcal{F}$ on which the basic observables of the theory are represented as annihilation and creation operators $P_n$. On the other hand, if the scalar field propagates in a globally hyperbolic spacetime, e.g. $\mathcal{M} \cong \Sigma \times \mathbb{R}^+$, given an embedding $\Sigma_0$ of $\Sigma$ as a Cauchy surface in $\mathcal{M}$ one gets, from the covariant complex structure $J$ on $V$, the induced complex structure $J_0$ on the canonical phase space $\Gamma$ 24. Once we have $J_0$, we know how to construct the Schrödinger representation which is unitarily equivalent to the Fock one 24 and how to pass from one representation to the other 25. In particular, we have the analog of the one-particle Hilbert space and, by applying the creation operator, one can construct the $n$ (functional) particle states.

In addition, as a consequence of this unitary relation between the covariant and canonical approaches, if a symplectic transformation is unitarily implementable with respect to the Fock representation, so is it with respect to the (unitarily equivalent) Schrödinger representation (and vice versa). Recall that a symplectic transformation on $V (\Gamma)$ will be unitarily implementable with respect to the Fock (Schrödinger) representation if the antilinear part of its quantum counterpart is Hilbert-Schmidt on the one-particle Hilbert space $\mathcal{H}$. For a quantum transformation of the Bogoliubov type, the Hilbert-Schmidt condition reduces to $\sum_{n,m} |\xi_{nm}|^2 < \infty$.

Consider now the Schrödinger representation constructed from $J_0$ (the complex structure induced by the covariant one, $J$). Given a symplectic transformation $T$ on $\Gamma$, we obtain an induced complex structure $J'_0 = T J_0 T^{-1}$ and, associated with it, a new Schrödinger representation. The annihilation and creation operators in this new representation are related with the annihilation and creation operators of the former one through a Bogoliubov transformation. The representations corresponding to $J'_0$ and $J_0$ are then unitarily equivalent if the antilinear part of this Bogoliubov transformation is square summable. In particular, if $T = T_{(t_1, t_2)}$ represents the time evolution from $t_1$ to $t_2$ on $\Gamma$, then the Bogoliubov transformation relates the annihilation and creation operators at the instants $t_1$ and $t_2$. With an appropriate choice of coordinates in $\Gamma$, the symplectic transformation $T_{(t_1, t_2)}$ acts on the elements of this space exactly as the Bogoliubov transformation on their quantum counterparts. Thus, in order to elucidate whether the symplectic transformation is unitarily implementable it suffices to analyze the square summability of the antilinear part of $T_{(t_1, t_2)}$.

Let us emphasize that this procedure is equivalent to determining whether the Schrödinger representations constructed from the same $\Gamma$ (associated with the embedding $\Sigma_0$) but with the distinct complex structures $J_1$ and $J_2$ are unitarily related.

In the following, we will focus our discussion on analyzing the failure of unitary implementability of the symplectic transformation that determines the dynamics in $\Gamma$, rather than examining the complex structures induced by it, since both procedures are equivalent, as we have just seen.

A. Evolution in the canonical and covariant approaches

We start by expanding in Fourier series our canonical variables $\phi$ and $P_\phi$:

$$\phi = \sum_{n \in \mathbb{Z}} \frac{1}{\sqrt{2\pi}} \phi_n e^{i n \theta}, \quad P_\phi = \sum_{n \in \mathbb{Z}} \frac{1}{\sqrt{2\pi}} P^n_\phi e^{i n \theta}.$$  

where the coefficients $\phi_n$ and $P^n_\phi$ are (implicit) functions of the global time coordinate. From the basic Poisson bracket between $\phi$ and $P_\phi$, it is easily shown that $\{\phi_n, P^m_\phi\} = \delta_{nm}$. Therefore, we can equivalently consider as our canonical phase space that whose coordinates are the set of (complex) canonical pairs $\{(\phi_n, P^n_\phi)\}_{n \in \mathbb{Z}}$. We will call it $\Gamma_{\phi, P_\phi}$. Note that this space can be decomposed as the direct sum of $\Gamma$ and $\Gamma_0$, where $\Gamma$ is the subspace of vectors with $\phi_0 = P^0_\phi = 0$ and $\Gamma_0$ is the span of those vectors whose only nonvanishing components are precisely those corresponding to $\phi_0$ and $P_0$. For

3 Let us emphasize that the coefficients in Eq. (22) do not display any time dependence, not only explicitly, but also implicitly. Accordingly, the total Hamiltonian in $V$ indeed vanishes. Properly speaking, the nonunitarity proved in Ref. 6 is that of the transformation generated by $H_r$ on $V$, which in turns can be seen to imply the nonunitary character of the dynamics in $\Gamma$, rather than in $V$. 


all positive integers \( m \in \mathbb{N} - \{0\} \), let us now consider the transformations
\[
(\phi_m, P_{\phi}^m, \phi_{-m}, P_{\phi}^{-m}) \mapsto (a_m, a_m^*, a_{-m}, a_{-m}^*) ,
\]
where
\[
a_m = \frac{|m|\phi_m + iP_{\phi}^m}{\sqrt{2|m|}} , \quad a_m^* = \frac{|m|\phi_{-m} - iP_{\phi}^{-m}}{\sqrt{2|m|}} .
\]
(27)

One can check that these transformations are canonical, so that \( [a_n, i\phi_m^*] = \delta_{nm} \). Hence, the canonical phase space can be alternatively described by the symplectic vector space \( \Gamma_a = \Gamma_0 \oplus \Gamma \), where the coordinates for \( \Gamma \) are the (complex conjugate pairs of) annihilation and creation-like variables \((a_m, a_m^*, a_{-m}, a_{-m}^*)\)\(_{m \in \mathbb{N} - \{0\}}\). The dynamics on \( \Gamma_a \) [as well as in \( \Gamma \) and \( \Gamma_{(\phi, P_\phi)} \)] is dictated by the reduced Hamiltonian for the polarized Gowdy \( T^3 \) model, \( H_\tau = \phi \cdot \mathcal{H}_\tau \), where \( \mathcal{H}_\tau \) is the reduced Hamiltonian density \([19]\). Using expressions \((25)\) and \((27)\), and defining
\[
H_0 := \frac{(p_0^0)^2}{2t} , \quad H_m := \frac{t}{2t} m (a_m a_m^* + a_{-m} a_{-m}^*) + \frac{t}{2t} m (a_m^* a_{-m} + a_{-m}^* a_m) ,
\]
(28)
the Hamiltonian can be rewritten
\[
H_\tau = H_0[p_\phi^0] + \sum_{m \in \mathbb{N}, m \neq 0} H_m[a_m, a_m^*, a_{-m}, a_{-m}^*] .
\]
(29)

Notice that the Hamiltonian vector field \( X_{\mathcal{H}_\tau} \) on \( \Gamma_a \) is just the sum of the Hamiltonian vector fields \( X_{H_0} \) on \( \Gamma_0 \) and \( X_{H_m} \) on \( \Gamma \), with \( H := \sum_{m \in \mathbb{N} - \{0\}} H_m \). In other words, for any state in \( \Gamma_a \), the time evolution can be deduced by composing the evolution of the projections in \( \Gamma_0 \) and in \( \Gamma \), where the dynamics are dictated, respectively, by \( H_0 \) and \( H \). In particular, we see that the unitary implementability of the dynamics in \( \Gamma_a \) at the quantum level depends only on whether the finite transformations generated by \( H_\tau \) on \( \Gamma_a \) can be unitarily implemented.

The covariant phase space \( \mathcal{V} \), on the other hand, can be described using as coordinates the canonical pair \((q_0, p_0)\) and the set of (complex conjugate) annihilation and creation-like variables \((a_n, a_n^*)\)\(_{n \in \mathbb{Z} - \{0\}}\). Let us denote the covariant phase space, in such a coordinate system, by \( V_\Lambda \). We can now separate the zero modes exactly as before, namely, \( V_\Lambda \) can be viewed as the direct sum of the subspace \( \tilde{V} \) for which \( q_0 = p_0 = 0 \) and the subspace \( V_0 \) whose vectors have \( q_0 \) and \( p_0 \) as the only nonzero components. In the following, we will respectively denote states in \( \Gamma_0 \) and \( V_0 \) by \( \psi_0 := (\phi_0, P_{\phi}^0) \) and \( \phi_0 := (\tilde{q}_0, \tilde{p}_0) \). Similarly, states in \( \tilde{\Gamma} \) and \( \tilde{V} \) will be denoted by \( \gamma_m := (a_m, a_m^*, a_{-m}, a_{-m}^*) \) and \( \mathcal{A}_m := (A_m, A_m^*, A_{-m}, A_{-m}^*) \), with \( m \in \mathbb{N} - \{0\} \).

Since \( \phi \) and \( P_\phi \) are the configuration and momenta at \( \Sigma_0 \) of \( \varphi \), we can express the coefficients \( \phi_m \) and \( P_{\phi}^m \) in terms of \( A_n \) and \( A_{-n} \) for all \( n \in \mathbb{Z} - \{0\} \), and in terms of \( \tilde{q}_0 \) and \( \tilde{p}_0 \) for the zero mode, getting in this way a map \( \tilde{M} \) from \( V_\Lambda \) to \( \Gamma_0 \). In addition, Eq. \((27)\) defines a map \( \tilde{M} \) from \( \Gamma_{(\phi, P_\phi)} \) to \( \Gamma_0 \). Then the composition \( \tilde{M} \tilde{M} \) provides us with a map \( M : V_\Lambda \to \Gamma_0 \). A straightforward calculation shows that for the zero modes
\[
u_0 = \left[ \begin{array}{cc} 1 & \ln t \\ 0 & 1 \end{array} \right] v_0 ,
\]
where \( u_0 \) and \( v_0 \) are treated as column vectors. For the rest of modes \((m \in \mathbb{N} - \{0\})\), one obtains \( \gamma_m = M_m(t) \mathcal{A}_m \) with
\[
M_m(t) = \left[ \begin{array}{ccc} c_m(t) & 0 & d_m(t) \\ 0 & c_m^*(t) & d_m^*(t) \\ 0 & d_m^*(t) & c_m(t) \end{array} \right] ,
\]
and
\[
c_m(t) = \sqrt{\frac{8}{r t}} \left[ H_0(mt) - it H_1(mt) \right] ,
\]
\[
d_m(t) = \sqrt{\frac{8}{r t}} \left[ H_0^*(mt) - it H_1^*(mt) \right] .
\]
Here, \( H_1 \) is the first-order Hankel function of the second kind \([21]\). Note that the map \( M \) is such that \( M(V_0) = \Gamma_0 \) and \( M(\mathcal{V}) = \Gamma \). Besides, the determinant of the linear transformation \((30)\), as well as that of \( M_m \), is equal to the unity. It hence follows that the \( M_m \)’s are Bogoliubov transformations. Thus, we get a time-dependent canonical transformation from \( V_\Lambda \) to \( \Gamma_\tau \).

A generating function for this transformation (that depends on some appropriately chosen complete sets of compatible components under Poisson brackets both for \( V_\Lambda \) and \( \Gamma_\tau \)) is
\[
\mathcal{F}_0(t) = \frac{1}{2} (p_0^0)^2 \ln t - \tilde{p}_0 \phi_0 ,
\]
\[
\mathcal{F}_m(t) = i a_m^* [c_m(t) A_m - d_m(t) A_{-m}^*] - i a_m [d_m^*(t) A_{-m}^* - c_m^*(t) A_{-m}^*] ,
\]
(33)
for \( m = 0 \) and \( m \in \mathbb{N} - \{0\} \), respectively. After a straightforward calculation we find that the partial derivative of this generating function with respect to its explicit dependence on the time coordinate \( t \) has the following form when expressed exclusively in terms of the components of the states in \( \Gamma_a \):
\[
\partial_t \mathcal{F}_0 = \frac{1}{2t} (p_\phi^0)^2 , \quad \partial_t \mathcal{F}_m = H_m[\gamma_m] .
\]
(34)
Therefore, we get
\[
\partial_t \mathcal{F}[u, \gamma] = \sum_{m \in \mathbb{N}} \partial_t \mathcal{F}_m[u, \gamma] = H_t[u, \gamma] ,
\]
(35)
where \( H_t \) is precisely the Hamiltonian \([22]\).

At this point of the discussion, it is worth recalling that, given a canonical transformation from certain symplectic vector space \( E_1 := \{(q, p)\} \) to another one \( E_2 := \{(Q, P)\} \) which is determined by a generating function \( F \) that is explicitly time dependent \([22]\), and assumed that the dynamics in \( E_1 \) is dictated by the Hamiltonian \( H_1[q, p] \), the corresponding Hamiltonian in \( E_2 \) is \( H_2[Q, P] = H_1[q (Q, P), P (Q, P)] + \partial_t F[Q, P] \).
Taking into account Eq. (25), we then see that the dynamical evolution in $\Gamma_m$, generated by $H_m$, arises entirely from the time dependence of the canonical transformation. As we have pointed out before, the total Hamiltonian in $V_{\tilde{m}}$ is identically zero and there is no time evolution for the states $(\gamma_m(t_0), \mathcal{A}_m)$. Obviously, this vanishing of the Hamiltonian applies as well to the restrictions to the subspaces $V_0$ and $\tilde{V}$. In particular, while the states in $\Gamma$ evolve along the integral curves of the Hamiltonian vector field $X^0$, the states in $\tilde{V}$ are "frozen". Hence, an initial state $(\gamma_m(t_0), t) \in \tilde{V}$ will evolve to the state $(\gamma_m(t), t)$ determined by the transformation $\gamma_m(t) = U^{(m)}_{H_{\tilde{m}}}(0, t)\gamma_m(0)$, where $\gamma_m(t)(t_0) := M_m(t_0)^{-1}$. In contrast, the corresponding states in $\tilde{V}$, specified by $\mathcal{A}_m(t_0) = M_m(t_0)^{-1} \gamma_m(t_0)$ and $\mathcal{A}_m(t) = M_m(t)^{-1} \gamma_m(t)$, will be related via the identity map, so that they actually coincide.

In coordinates $\mathcal{A}_m$ rather than $\gamma_m$, the finite transformation $U^{(m)}_{H_{\tilde{m}}}(t_0)$ is given by $U^{(m)}_{H_{\tilde{m}}}(t_0) = (M_m(t_0)^{-1})^{-1}$. As a result, the complex antilinear part of the finite transformation generated by $H = H_f - H_0$ in $\tilde{V}$ is given (for each $m \in \mathbb{N} - \{0\}$) by

$$D_m(t, t_0) = \frac{i m}{4} [t_0 H^*_m(m_0) H^*_m(m t) - t H^*_m(m t_0) H^*_m(m t)], \quad (36)$$

which is not square summable in $m$, as has been proved in Ref. [6]. Therefore, the finite transformation provided by $M_m(t_0)^{-1} M_m(t)$ (with $m$ running in $\mathbb{N} - \{0\}$) cannot be unitarily implemented. Moreover, since the antilinear part of $U^{(m)}_{H_{\tilde{m}}}(t, t_0)$ differs from that of $U^{(m)}_{H_{\tilde{m}}}(t_0, t_0)$ just by a sign in the phase of the coefficient $c_m(t)$, as one can easily check, we see that the finite transformation generated by $H$ in $\tilde{V}$ is not unitarily implementable. It is worth emphasizing that, however, this is not the case for the dynamics in $\tilde{V}$; indeed, since such a dynamics is generated by the zero Hamiltonian, the evolution is described by the identity transformation, which is of course unitary.

Actually, $U^{(m)}_{H_{\tilde{m}}}(t_0, t_0)$ is just a composition of the Bogoliubov transformations $M_m(t)$ and $M_m(t_0)$, the lack of a unitary implementation of the dynamics in $\tilde{V}$ follows from the fact that the antilinear part of $M_m(t)$ fails to be square summable for generic $t > 0$. Hence, whether or not the dynamics can be unitarily implemented depends entirely on the behavior of $d_m(t)$ for large integers $m$. This depends in turn on the Hamiltonian via Eq. (24), which relates the generating function of $M_m(t)$ with the generator of the dynamics after the canonical transformation has been performed. Our analysis about the lack of unitarity will therefore focus on the identification of those characteristics of the Hamiltonian that are in the origin of the failure of square summability. In doing so, we will be able to establish how critical this problem is and whether it can be corrected with small modifications to the dynamics. Roughly speaking, we will be able to determine how far the considered evolution is from being unitarily implementable.

With this aim, in the next subsection we introduce a correction to the Hamiltonian $H$, which might be viewed as a perturbation or a quantum modification, and discuss the square summability of the antilinear part of the transformation generated by the new Hamiltonian.

### B. Modified Hamiltonian

Motivated by our previous analysis, let us assume now that a certain linear (free) field theory can be described by either of the two symplectic vector spaces $E_A := \{\mathcal{A}_m\}$ or $E_B := \{B_m\}$, where $\mathcal{A}_m := \{A_m, A^*_{-m}, A_{-m}, A^*_m\}$, $B_m := \{B_m, B^*_{-m}, B_{-m}, B^*_m\}$, and $m \in \mathbb{N} - \{0\}$. Here, $(A_m, A^*_m)$ and $(B_m, B^*_m)$ are annihilation and creation-like pairs. In addition, let us suppose that the canonical map $M_m(t)$ from $E_A$ to $E_B$, which in general may depend on the time coordinate $t$, is a Bogoliubov transformation of the form (31), with $|e_m(t)|^2 - |d_m(t)|^2 = 1$. Besides, we assume that the total Hamiltonian in $E_B$ is zero, so that the Hamiltonian in $E_B$ is given by $H = \sum_{m \in \mathbb{N} - \{0\}} \partial_t F_m$, where $F_m$ is a generating function of the transformation $M_m(t)$. Furthermore, we admit that (in coordinates $\mathcal{A}_m$) the partial derivative of the generating function $F_m$ with respect to its explicit time dependence is

$$\partial_t F_m = R_m[\mathcal{A}] := 2m [\mu a(x)A_m A^*_m + \mu' a^*(x)A^*_m A_m] + 2m \lambda(b(x)A^*_m A_m + A^*_m A_m A_m), \quad (37)$$

where $x := mt$ (strictly speaking we should write $x_m$, however we drop out the subindex to simplify the notation). Besides, $\lambda$ and $\mu$ are a real and a complex constant, respectively, and

$$a(x) = \sqrt{\frac{\pi}{8}} \left[[H_0(x)]^2 + [H_1(x)]^2\right],$$

$$b(x) = \sqrt{\frac{\pi}{8}} \left[[H_0(x)]^2 + [H_1(x)]^2\right]. \quad (38)$$

At this stage, it is convenient to point out the analogy with our symmetry-reduced model. The Bogoliubov transformation $M_m(t)$ has the same form as that in Eq. (31). The symplectic vector spaces $E_A$ and $E_B$ play the role of $\tilde{V}$ and $\tilde{\Gamma}$, respectively. In this sense, note that the total Hamiltonian in $E_A$ is zero. Moreover, setting $\lambda = \mu = 1$ in equation (37) one merely gets the contribution to the total Hamiltonian $H$ in $\tilde{\Gamma}$, expressed in coordinates $\mathcal{A}_m$ [7]. Hence, we can think in terms of the spaces $\tilde{V}$ and $\tilde{\Gamma}$, and regard the phase space function $H$ as a modification of the Hamiltonian $H$. Defining $\rho := \lambda - 1$ and $\epsilon = \mu - 1$, one may view the case $|\rho| < 1$, $|\epsilon| < 1$ as a perturbation of the Hamiltonian, arising from certain (classical or quantum) corrections to the dynamics.

As we already know, the unitary implementability of the dynamics dictated by $H$ in $E_B$ depends on the square summability of the antilinear part of $M_m(t)$. By analyzing this

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4 Actually $U^{(m)}_{H_{\tilde{m}}}(t_0, t_0) = 1$ and $U^{(m)}_{H_{\tilde{m}}}(t_2, t_1) = U^{(m)}_{H_{\tilde{m}}}(t_1, t_2) U^{(m)}_{H_{\tilde{m}}}(t_2, t_1)$.外

5 We might allow for an $x$-dependence in $\lambda$ and $\mu$, but this would unnecessarily complicate our discussion. Some comments about this generalization of the analysis are presented in Subsec. III.C.
summability we will relate the failure of unitarity with the precise form of \( \mathcal{H} \).

We first determine the relations that Eq. \( (\text{m}) \) imposes on the complex functions \( c_m(t) \) and \( d_m(t) \) that specify the Bogoliubov transformation \( M_m(t) \). A generating function for this transformation is

\[
\mathcal{F}_m(t) = i B_m c_m(t) A_m + d_m(t) A_m^* - i B_m^* d_m(t) A_m^*.
\]

Taking the (explicit) time derivative and using then the inverse of \( M_m(t) \), one arrives at the following expression, exclusively in terms of the coordinates \( B_m \),

\[
\partial_t \mathcal{F}_m = i B_m^* B_m (c_m c_m^* - d_m d_m^*) + i B_m B_m (c_m^* d_m^* - d_m c_m)
+ i B_m^* B_m d_m c_m + i B_m^* B_m^* d_m^* c_m.
\]

The dot denotes the (total) derivative with respect to the time coordinate \( t \). From now on, we do not generally display the dependence of \( c_m \) and \( d_m \) on this coordinate in order to simplify the notation.

By translating also into coordinates \( B_m \) the Hamiltonian \( \mathcal{H}_m \), the condition \( (\text{m}) \) that the dynamics in \( E_\beta \) arise entirely from the time derivative of our canonical transformation can be seen to reduce to the following system of first-order (complex) differential equations for \( c_m \) and \( d_m \):

\[
0 = \frac{i}{\sqrt{2}} (c_m^* c_m - d_m d_m) + m \lambda b(x) \left( |c_m|^2 + |d_m|^2 \right) - m [\mu a(x) c_m d_m^* + \mu^* a^*(x) c_m^* d_m],
\]

\[
0 = \frac{i}{\sqrt{2}} (d_m c_m - c_m^* d_m) + 2m \lambda b(x) c_m d_m + m [\mu a(x) c_m^* + \mu^* a^*(x) c_m].
\]

Let us call \( Y_m \) the ratio \( d_m/c_m \). Since \( |c_m|^2 - |d_m|^2 = 1 \), we have that \( |Y_m|^2 = |c_m|^2 \) strictly smaller than the unity and, in terms of it, the (complex) norms of \( c_m \) and \( d_m \) are

\[
|c_m|^2 = \frac{1}{1 - |Y_m|^2}, \quad |d_m|^2 = \frac{|Y_m|^2}{1 - |Y_m|^2}.
\]

Realizing that \( (d_m c_m - c_m^* d_m)/c_m^2 \) is just the time derivative of \( Y_m \) and performing the change of variable \( t \to x = mt \) (so that \( Y_m = m dY_m/dx \)), it is easy to see that Eq. \( (\text{m}) \) can be rewritten as

\[
\frac{i}{\sqrt{2}} \frac{dY_m}{dx} + 2 \lambda b(x) Y_m - \mu a(x) Y_m^2 - \mu^* a^*(x) = 0.
\]

Remarkably, this differential equation for \( Y_m \) is independent of the positive integer \( m \) (regarding \( x \) as the relevant variable). Using this universal character of the equation, valid for all values of \( m \), we can drop out the subindex in the function \( Y_m \) and consider it as a single function \( Y \) for all the modes of our system. With the convenient redefinitions

\[
z(x) := \exp(-2ix) Y \), \quad \Delta(x) := \exp(2ix) a(x),
\]

we then arrive at the following equation for \( z \):

\[
\frac{dz}{dx} = 2iz(z) [2 \lambda b(x) - 1] - 2i \mu \Delta(x) z^2(x) - 2i \mu^* \Delta^*(x).
\]

In addition, given a function \( \zeta \) satisfying Eq. \( (\text{m}) \) and remembering that \( |c_m|^2 - |d_m|^2 = 1 \), it is straightforward to see that the differential equation \( (\text{m}) \) is equivalent to

\[
\frac{d}{dx} \ln c_m(x) = 2i [\mu \Delta(x) \zeta(x) - \lambda b(x)]
\]

which again is a universal equation for all modes \( m = \mathbb{N} \). We suppress the subindex \( m \) and consider only one function \( \zeta(x) \), which can be obtained by direct integration of Eq. \( (\text{m}) \) [except for a multiplicative constant that can be fixed with an initial condition for \( \zeta \)]. Finally, the function \( d(x) := \exp(2ix) \zeta(x) \zeta(x) \) provides the missing coefficient of our Bogoliubov transformation, namely, \( d_m(t) = d(x = mt) \).

Using Eq. \( (\text{m}) \) and \( |Y(x)| = |\zeta(x)| \), we conclude

\[
|d_m(t)|^2 = |d(x = mt)|^2 = \frac{|\zeta(x = mt)|^2}{1 - |\zeta(x = mt)|^2}.
\]

Therefore, an important consequence of the observed universality is that the square summability of the coefficients \( d_m(t) \) at any fixed positive value of \( t \), which is only sensitive to the behavior for large \( m \), turns out to depend exclusively on the behavior of the function \( \zeta(x) \) when \( x \) approaches infinity (because \( x = mt \) grows linearly with \( m \) for all \( t > 0 \)). Thus, to discuss the square summability of \( d_m \), we only need to consider Eq. \( (\text{m}) \) and exploit our knowledge about the asymptotic behavior of the functions \( \Delta(x) \) and \( b(x) \).

From Hankel’s asymptotic expansions of \( H_0 \) and \( H \), one gets that, for \( x \gg 1 \), \( \Delta(x) \) and \( b(x) \) are given by the asymptotic series

\[
\Delta(x) = \frac{i}{\sqrt{2}} \sum_{k,n=0}^{\infty} \left( -1 \right)^{k+n} \frac{(2k+n)!}{(2k)! (2n)!} \left( \xi_{k,n} - i \xi_{k,n+1/2} \right) \left( \frac{x^{2(k+n)}}{4x^2} - \frac{x^{2k+1/2}}{2x^2} \right),
\]

\[
b(x) = \frac{1}{\sqrt{2}} \sum_{k,n=0}^{\infty} \left( -1 \right)^{k+n} \frac{(2k+n)!}{(2k)! (2n)!} \left( \sigma_{k,n} + i \sigma_{k,n+1/2} \right) \left( \frac{x^{2(k+n)}}{4x^2} - \frac{x^{2k+1/2}}{2x^2} \right)
\]

where

\[
\xi_{k,n} := (0, 2k)(0, 2n) - (1, 2k)(1, 2n),
\]

\[
\sigma_{k,n} := (0, 2k)(0, 2n) + (1, 2k)(1, 2n),
\]

and \((k, n)\) is the so-called Hankel symbol:

\[
(k, n) := \frac{\Gamma \left( k + n + \frac{1}{2} \right)}{n! \Gamma \left( k - n + \frac{1}{2} \right)}.
\]

The asymptotic series representation for \( b(x) \) contains only even powers in \( 1/x \), while the corresponding asymptotic series for \( \Delta \) contains, in principle, both even and odd powers. With

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6 In general, we will say that a function \( f \) admits an asymptotic series at infinity if there exists a series of the form \( \sum_{i=0}^{\infty} \frac{f_k}{x^k} \) such that \( \lim_{x \to \infty} \left| x^N \left( f(x) - \sum_{i=0}^{N} \frac{f_k}{x^k} \right) \right| = 0 \) for all \( N \geq 0 \) (see e.g. Ref. [28]).
the change of variable $y = 1/x$, these asymptotic expansions can thus be written in the form

$$
\Delta(y) = \sum_{k=0}^{\infty} \Delta_k y^k, \quad b(y) = \sum_{k=0}^{\infty} b_k y^k,
$$

(52)

where $b_{2k+1} = 0$ for all $k \in \mathbb{N}$. From Eqs. (49), we get in particular

$$
\Delta_0 = \frac{\xi_{0,0}}{4} = 0, \quad \Delta_1 = \frac{\xi_{0,1/2}}{4} = -\frac{1}{4},
$$

$$
b_0 = \frac{\sigma_{0,0}}{4} = \frac{1}{2}.
$$

Employing the asymptotic expressions for $\Delta(x)$ and $b(x)$, a formal asymptotic series for $z$ can be constructed. More precisely, introducing expansions (52) in the differential equation (46) (with the change $y = 1/x$) and writing $z$ as an asymptotic series in $y$, namely $z = \sum_{k=1}^{\infty} z_k y^k$, one obtains

$$
z_0^2 \mu \Delta_0 + z_0 (1 - 2 \lambda b_0) + \mu^* \Delta_0^* + \sum_{k=1}^{\infty} y^k S_k = 0,
$$

(54)

where, for each $k \geq 1$, $S_k := \mu \sum_{m=0}^{k} \Delta_k - \sum_{j=0}^{m} z_{m-j} z_j - 2 \lambda \sum_{m=0}^{k} b_m z_{k-m} + z_k + \mu^* \Delta_k^* + i \frac{k-1}{2} z_{k-1} + \mu \Delta_k z_k^2.
$$

(55)

In particular, the term independent of $y$ in Eq. (52) must vanish. Since $b_0 = 1/2$ and $\Delta_0 = 0$, one gets (with $\rho = \lambda - 1$)

$$
z_0 \rho = 0.
$$

(56)

Hence, provided that $\rho$ does not vanish, the coefficient $z_0$ must be zero. As a consequence, the resulting function $z$ will tend to zero as $x \to \infty$, which in turn implies that $|d|$ vanishes in the limit of large values of $x$.

The rest of terms in Eq. (54) require the vanishing of $S_k$ for all $k \geq 1$. Substituting the values of $b_0$ and $\Delta_0$, it is straightforward to derive the following recurrence relation for the complex coefficients of the asymptotic series of $z$:

$$
z_k = \frac{1}{\rho} \left[ \sum_{m=0}^{k-1} \Delta_k - \sum_{j=0}^{m} z_{m-j} z_j - 2 \lambda \sum_{j=0}^{k} b_m z_{k-m} \right] + \frac{1}{\rho} \left[ \mu^* \Delta_k^* + i \frac{k-1}{2} z_{k-1} \right].
$$

(57)

For the first coefficient, we get $z_1 = \mu^* \Delta_1^*/\rho = -\mu^*(4 \rho)$. Thus, for sufficiently large values of $x$, the differential equation (46) should admit a solution $z$ such that

$$
z(x) = \left( \frac{\mu^*}{4 \rho} \right) x + \theta \left( \frac{1}{x} \right).
$$

(58)

As we will see, this result suffices to prove the square summability of the coefficients $d_m$. Of course, the above behavior is not allowed for $z$ when $2b_0 \lambda - 1 = \rho$ vanishes, as it is the case for the Hamiltonian $H$. This explains the break down of unitarity for that specific case.

### C. Unitarity of the Modified Dynamics

Let us finally show that the deduced asymptotic behavior for $z(x)$, together with relation (48), guarantee the square summability of the sequence $\{d_m(t)\}$ for all fixed, strictly positive values of the time coordinate $t$. From Eq. (58), we see that, at infinity, $\lim_{x \to \infty} |x z + \mu^*/(4 \rho)| = 0$. So, given any constant $\varepsilon > 0$ there exists a positive number $x_0(\varepsilon)$ such that $|x z + \mu^*/(4 \rho)| < \varepsilon$ for all $x > x_0(\varepsilon)$. One can see that this inequality implies that, for all $x > x_0(\varepsilon)$,

$$
|z|^2 < \frac{R(\varepsilon, \rho, \mu)}{x^2}, \quad R(\varepsilon, \rho, \mu) := 2 \varepsilon^2 + 8 \varepsilon |\mu|/|\rho| + \frac{|\mu|^2}{16 \rho^2}.
$$

(59)

Let us now choose a number $\tilde{x}_0$ in the interval $(x_0(\varepsilon), \infty)$ such that $\eta_0 := R(\varepsilon, \rho, \mu)/x_0^2 < 1$, which is clearly always possible. Then, for all $x > \tilde{x}_0$,

$$
|z|^2 < \frac{R(\varepsilon, \rho, \mu)}{x^2} < \eta_0 < 1.
$$

(60)

Therefore, for all $x > \tilde{x}_0$ we have

$$
|z|^2 < \frac{R_0}{x^2}, \quad R_0 := \frac{R(\varepsilon, \rho, \mu)}{1 - \eta_0}.
$$

(61)

Notice that $R_0$ is a finite and strictly positive constant. Employing Eq. (58) and this inequality, we obtain that for all $m > M_0 := \text{int}(\tilde{x}_0/t) + 1$ (where $\text{int}(x)$ is the integer part of $x$)

$$
|d(m t)|^2 < \frac{R_0}{(m t)^2}.
$$

(62)

Therefore, we conclude that, for every fixed $t > 0$,

$$
\sum_{m \in \mathbb{N}} |d(m t)|^2 < \sum_{m=1}^{M_0} |d(m t)|^2 + \frac{R_0}{t^2} \sum_{m=M_0+1}^{\infty} \frac{1}{m^2} < \frac{M_0}{6 t^2} + \frac{\pi^2 R_0}{6 t^2} < \infty.
$$

(63)

Thus, $d_m$ is square summable, and the dynamics generated by $\tilde{H}$ in $E_{cb}$ is unitarily implementable. The proof, which makes use of Eq. (58), fails when $\rho = 0$ and, in particular, for the Hamiltonian $H$. We hence see that unitary implementability is extremely sensitive to the value of $\rho$. For instance, for every nonvanishing real $\rho$ in any neighborhood of zero (in fact, for all $\rho \in \mathbb{R} \setminus \{0\}$, $R_m[A] = H_m[A] + 2 m b \rho t (x)(A^*_x A_m + A^*_m A_x)$ gives rise to a unitarily implementable transformation.

On the other hand, it is worth emphasizing that, to prove the square summability of $d_m$, we have not actually employed the existence of an asymptotic series for a solution $z$ of Eq. (46). What we have used in fact is a weaker property, namely,

---

A function $f(x)$ is $o(1/x^2)$ at infinity if $\lim_{x \to \infty} x^2 f(x) = 0$.
the existence of a solution with the behavior \( \beta(x) \). A rigorous proof of this existence is given in the appendix.

In our analysis, we have assumed a specific form for the Hamiltonian, in particular that \( \lambda \) and \( \mu \) are a real and a complex constant. It is nonetheless possible to generalize our discussion to other cases. Suppose, e.g., that the function \( \lambda(x) \) is replaced by a new real function \( \tilde{\lambda}(x) \) and that \( \mu(x) \) is changed into \( \tilde{\mu}(x) := \exp[-2i\phi(x)]\tilde{\lambda}(x) \) (and similarly for its complex conjugate), with \( \phi \) and \( \tilde{\lambda} \) being a real and a complex function, respectively. Let us then call \( \tilde{\beta}(x) := 2\tilde{\lambda}(x) - i\tilde{\mu}(x)/dx \) and assume that \( \tilde{\beta}(x) \) and \( \tilde{\lambda}(x) \) admit asymptotic series at infinity such that \( \tilde{\lambda}_0 = 0 \). Defining now \( \tilde{z}(x) = \exp[-2i\phi(x)]Y(x) \), it is straightforward to see that the same line of reasoning presented in the previous subsection leads to an equation analogous to Eq. \((46)\), but with the replacements of \( z \) by \( \tilde{z} \), \( 2ib - 1 \) by \( \tilde{\beta} \), and \( \mu \Delta \) by \( \tilde{\lambda} \). The counterpart of Eq. \((50)\) is then \( \tilde{z}_0 = 0 \), which implies that \( \tilde{z}_0 \) vanishes unless so does \( \tilde{\beta}_0 \), which plays now the role of \( \rho \). In addition, the analog of Eq. \((57)\) is

\[
\tilde{z}_k = \frac{1}{\tilde{\beta}_0} \left[ \sum_{m=0}^{k-1} \tilde{\lambda}_{k-m} \left( \sum_{j=0}^{m} \tilde{z}_{m-j} \right) - \sum_{m=1}^{k} \tilde{\mu}_{m+k-m} \right] + \frac{1}{\tilde{\beta}_0} \tilde{\lambda}^*_k i - \frac{1}{2} \tilde{z}_{k-1}.
\]

Therefore, we get \( \tilde{z}(x) = \tilde{\lambda}_1/(2\tilde{\beta}_0) + o(1/x) \). Again, this asymptotic behavior suffices to guarantee the square summability of the antilinear part of the map \( M_m(t) \) for all \( t > 0 \) provided that \( \tilde{\beta}_0 \) differs from zero.

As a final comment, let us consider the formal quantum expression for \( \tilde{H} \):

\[
\tilde{H} := \tilde{H} := 2\rho \sum_{m} m b(m) \left[ \tilde{A}_m^\dagger \tilde{A}_m + \tilde{A}_m^{\ast \dagger} \tilde{A}_m \right].
\]

Because of the unitary implementability of \( M_m(t) \), we know that \( \tilde{H} \) generates the unitary evolution operator through which the basic operators \( \tilde{B}_n \) and \( \tilde{B}_n^\dagger \) evolve (when these basic operators are represented as the annihilation and creation operators on the Hilbert space \( \mathcal{H}_B \) constructed from \( E_B \) and its corresponding complex structure \( J_B \)). On the other hand, even though the operator \( \tilde{H} \) generates a map which acts unitarily on the Hilbert space \( \mathcal{H}_I \) (constructed from \( \tilde{\Gamma} \) and its associated complex structure \( J_I \)), we know that this map does not correspond to the actual time evolution of the basic operators \( B_n \) and \( B_n^\dagger \) (now represented as the annihilation and creation operators on \( \mathcal{H}_I \)). The quantum generator comes from a phase space function which certainly can be considered as close as one wants to \( H \) (the generator of the dynamics in \( \tilde{\Gamma} \)), but does not coincide with it. Nevertheless, it is interesting to note that if \( \rho \) is regarded as a constant of quantum origin, e.g. by setting \( \rho \) proportional to \( h \), then the classical limit of \( \tilde{H} \) would be just \( H \). That is, in spite of the lack of a unitary implementation for \( H \), if we consider that the modification of the Hamiltonian arises from a quantum correction, then we will get a unitary map whose generator, in the naive limit \( h \to 0 \), provides the classical dynamics in \( \Gamma \).

### IV. CONCLUSIONS AND FURTHER COMMENTS

We have analyzed the impossibility of obtaining a unitary implementation of the dynamics in the polarized Gowdy \( T^3 \) model with the quantization put forward in Ref. \( [5] \), a problem that has recently been pointed out in Refs. \( [6] \) and \( [7] \). With this aim, we have first presented a complete derivation of the model starting with general relativity and introducing a symmetry-reduction and gauge-fixing procedure. Employing then a time-dependent map from the covariant phase space to the canonical phase space of the system, we have been able to reformulate the issue of unitary implementability of the evolution as a question about the square summability of the antilinear part of such a map. In this process, it is important to realize that the total Hamiltonian in the covariant phase space vanishes, whereas the considered map includes in an explicit manner all of the time variation of the system. Exploiting this reformulation of the unitarity problem, we have considered (certain types of) modifications to the dynamics and analyzed whether the symplectic maps associated with them are unitarily implementable. In this way, we have traced back the failure of unitarity to the presence of some specific contributions in the Hamiltonian that generates the dynamics. In addition, we have seen that negligibly small modifications of these contributions suffice to restore unitarity. In the rest of the section, we present some comments about the main results of the work.

In our analysis, two facts have played a particularly relevant role. Firstly, as we have noticed, there is some kind of universality in the behavior of the Bogoliubov coefficients. This has allowed us to consider just one equation [namely Eq. \((46)\)] in order to examine the square summability of these coefficients, rather than investigating an infinite number of differential equations, one for each mode. Secondly, to know whether the modified Hamiltonian is unitarily implementable, instead of solving the universal equation \((46)\), it actually suffices to study the leading term of the function \( z \) in the asymptotic limit of large values of its argument. In this sense, one does not need to explicitly integrate the dynamical equations.

On the other hand, we note that solving Eq. \((42)\) amounts to “diagonalizing” the total Hamiltonian by means of a time-dependent canonical transformation, namely, to requiring that the terms proportional to \( B_n B_{-n}^\dagger \) and \( B_n^\dagger B_{-n} \) vanish in the phase space function \( \hat{H}(\mathcal{B}) := \hat{H}(\mathcal{B}) - \partial/\partial \mathcal{J}(\mathcal{B}) \). Had we ignored the term containing the time derivative of the Bogoliubov coefficients, we would have obtained from Eq. \((42)\) an algebraic quadratic equation for the ratio \( Y(x) \) of the coefficients that leads to an instantaneous diagonalization (i.e., at a fixed instant of time) of the Hamiltonian \( \hat{H} \). In fact, for \( \lambda = \mu = 1 \) so that \( \hat{H} \) reduces to \( H \), one can see that using this algebraic equation and the relation \( |c|^2 = 1 + |d|^2 \), it is possible to recover the instantaneous diagonalization given in Ref. \( [6] \). In addition, we emphasize that diagonalizing the Hamiltonian is equivalent to the resolution of the dynamics. Indeed, as we have seen, if we solve the universal equation \((46)\), which is equivalent to the diagonalization condition \((42)\), then \( c(x) \) can be found by simple integration of the first-order differential equation \((47)\), whereas \( d(x) \) is determined as \( d(x) = \exp(2ix) z(x)c(x) \).
Our discussion can be extended to Hamiltonians for which the functions \( \mu a(x) \) and \( \lambda b(x) \) in Eq. (37) are replaced by more general functions \( \bar{a}(x) \) and \( \bar{b}(x) \). We have seen that this is the case at least if \( \bar{a}(x) \) is of the form \( \exp \{-2i\psi(x)\bar{\Delta}(x)\} \) with \( \psi(x) \) real, and \( \bar{\Delta}(x) \) and (the real function) \( \bar{\beta}(x) := 2\bar{h}(x) - d\psi(x)/dx \) admit asymptotic series with a vanishing coefficient \( \bar{\Delta}_0 \). More precisely, we have proved that the dynamics generated by those Hamiltonians can be implemented as a unitary transformation as far as the coefficient \( \bar{\beta}_0 \) differs from zero. In this sense, our study provides a general treatment for Hamiltonians of the form (37), quadratic in the coordinates.

In this appendix, we want to prove that Eq. (46) admits one solution which, at infinity, has the asymptotic behavior \( \bar{\psi} \), provided that \( \rho \neq 0 \). Let us start by defining a new function \( w(x) \) by means of the relation

\[
\bar{z}(x) = \frac{\mu^*}{4\rho x} + \frac{w(x)}{x},
\]

Substituting this expression in Eq. (49) we obtain an equivalent nonlinear differential equation of the Riccati type

\[
\frac{dw}{dx} = w(x)\bar{\beta}(x) - 2\mu\frac{\Delta(x)}{x} w^2(x) + \alpha(x),
\]

where

\[
\bar{\beta}(x) := \frac{2i}{x} [2\lambda b(x) - 1] + \frac{1}{x} + i \frac{\mu^2}{\rho} \Delta(x),
\]

\[
\alpha(x) := -2i\mu x [\Delta^*(x) - \Delta^*_1] - i \frac{\mu\lambda}{\rho} [b(x) - b_0]
\]

\( - \frac{\mu^*}{4\rho x} - i \frac{\mu^* |\mu|^2}{8\rho^2} \Delta(x)/x \).

The constants \( \Delta_1 \) and \( b_0 \) are given in Eq. (52) and we have used \( \lambda = 1 + \rho \).

In order to arrive at the desired result about the asymptotic behavior of \( \bar{z}(x) \), we only have to demonstrate that Eq. (A2) admits a solution that tends to zero at infinity.

Employing the asymptotic expansions of the functions \( \Delta(x) \) and \( b(x) \), recalling that \( \Delta_0 = b_1 = 0 \), and making use of Eq. (49) to compute the coefficient \( \Delta_2 = i/16 \), one can rewrite

\[
\bar{\beta}(x) = 2i\rho + \frac{1}{x} + \bar{\beta}(x),
\]

\[
\alpha(x) = \left(1 - \frac{1}{2\rho}\right) \frac{\mu^*}{4x} + \bar{\alpha}(x),
\]

with \( \bar{\alpha}(x) \) and \( \bar{\beta}(x) \) being \( O(1/x^2) \) at infinity [we say that a function \( f(x) \) is \( O(1/x^3) \) at infinity if \( |x^n f(x)| \) admits a finite limit when \( x \to \infty \)]. Explicitly, these functions are

\[
\bar{\beta}(x) := \frac{4i}{\rho} \left[ (2\lambda b(x) - b_0) + i \frac{\mu^2 |\mu|^2}{\rho} \Delta(x)/x \right],
\]

\[
\bar{\alpha}(x) := -2i\mu x \left[ (\Delta^*(x) - \Delta^*_1) - \frac{\mu \lambda}{\rho} [b(x) - b_0] \right] - i \frac{\mu^* |\mu|^2}{8\rho^2} \Delta(x)/x .
\]

On the other hand, the function \( \Delta(x)/x \) that multiplies \( w^2(x) \) in Eq. (A2) is also \( O(1/x^2) \) asymptotically. For solutions \( w(x) \) that are small at infinity, we then expect the quadratic term in our Riccati equation to be negligible. We will hence approximate our equation by a linear one that can be explicitly solved, find for it a solution that tends to zero at infinity, and prove that, for that solution, the removed quadratic term can in fact be neglected in the original differential equation.

For the linear differential equation

\[
\frac{dw_1}{dx}(x) = w_1(x)\beta(x) + \alpha(x)
\]

APPENDIX A: PROOF OF THE ASYMPTOTIC BEHAVIOR

In this appendix, we want to prove that Eq. (46) admits one solution which, at infinity, has the asymptotic behavior \( \bar{\psi} \), provided that \( \rho \neq 0 \). Let us start by defining a new function

\[
\bar{z}(x) = \frac{\mu^*}{4\rho x} + \frac{w(x)}{x},
\]
all solutions can be constructed starting with those of the associated homogeneous equation. Using Eq. (A4), the homogeneous solutions can be found to be proportional to

$$w_l^0(x) = \frac{1}{2} \left[ 2i \mu x + \int_0^\infty d\bar{x} \frac{\alpha(\bar{x})}{2i \mu + \beta(\bar{x})} \right]. \quad (A7)$$

Note that the asymptotic behavior of $\beta$ guarantees that the integral that appears in this expression is well-defined. Solutions to Eq. (A4), modulo the possible addition of a complex constant, are then of the form

$$w_l(x|x_0) = w_l^0(x) \int_{x_0}^x d\bar{x} \frac{\alpha(\bar{x})}{w_l^0(\bar{x})}. \quad (A8)$$

where $x_0$ is a constant. A convenient integration by parts leads then to

$$w_l(x|x_0) = w_l^0(x) \int_{x_0}^x d\bar{x} \frac{\alpha(\bar{x})}{w_l^0(\bar{x}) \left( 2i \mu + \beta(\bar{x}) \right)} - \frac{\alpha(x)}{2i \mu + \beta(x)}. \quad (A9)$$

Remembering that $\alpha(x)$, $\beta(x)$, and $w_l^0(x)/x$ are respectively $O(1/x)$, $O(1/x^2)$ and $O(1)$ at infinity, it is possible to see that the integrand in the above expression is $O(1/x^3)$. Therefore, the integral converges when $x_0$ tends to infinity.

In that limit, one gets the particular solution

$$w_l^I(x) = w_l^I(x) \int_0^x d\bar{x} \frac{\alpha(x)}{w_l^0(\bar{x})} \left[ \frac{\alpha(\bar{x})}{2i \mu + \beta(\bar{x})} \right] x.$$\hspace{1cm} (A10)

One can see (e.g. using L’Hôpital’s rule for the term containing the integral) that this solution tends to zero when $x \to \infty$. Furthermore, repeating the explained procedure of integration by parts, one can show that the total contribution to $w_l^I(x)$ coming from the factor that includes the integral is $O(1/x^2)$. Using Eq. (A4), one then concludes that the asymptotic behavior of $w_l^I(x)$ is

$$w_l^I(x) = \left( 1 - \frac{1}{\rho} \right) \frac{\mu^*}{8i \mu x} + o \left( \frac{1}{x} \right). \quad (A11)$$

It now is a simple exercise to check that, in the Riccati equation (A2), the quadratic term is $O(1/x^3)$ at infinity for the solution $w_l^I(x)$, which is in fact negligible when compared with the rest of terms in the equation (in particular with $dw/dx$), which are at least of order $1/x^2$. This concludes our proof.