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Loop quantum cosmology evolution operator of an FRW universe with a positive cosmological constant

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The self-adjointness of an evolution operator Θ_Λ corresponding to the model of the flat FRW universe with massless scalar field and cosmological constant quantized in the framework of loop quantum cosmology is studied in the case $\Lambda > 0$. It is shown that, for $\Lambda < \Lambda_c \approx 10.3\ell_{\rm Pl}^{-2}$, the operator admits many self-adjoint extensions, each of the purely discrete spectrum. On the other hand for $\Lambda \geq \Lambda_c$ the operator is essentially self-adjoint, however the physical Hilbert space of the model does not contain any physically interesting states.

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I. INTRODUCTION

Among various approaches to the unification of general relativity and quantum physics, loop quantum gravity (LQG) [1,2] is one of the most promising. Its symmetry reduced version, loop quantum cosmology [3], offers a qualitatively new picture of an early universe evolution [4] and may provide a mechanism of solving long-standing problems in modern cosmology [5,6]. However, although the number of works using the heuristic methods of mimicking the quantum evolution by an appropriately constructed classical mechanics [7] is rapidly growing, not so much effort has been dedicated so far to the investigation on a genuinely quantum level. The rigorous studies of these aspects are in fact restricted just to models either *in vacuo* [8,9], or admitting massless scalar field as the only matter content [10–13]. The number of works attempting to include the cosmological constant Λ is even smaller [14] and the rigorous analysis of the quantum universe dynamics within the precise loop quantum cosmology (LQC) model [15] was done only for negative Λ, a case not favored by the observations.

This article is an attempt to partially fill this gap, by addressing the question of whether, in the presence of the *positive* cosmological constant, the physical evolution defined by the methods currently applied in LQC [16] is unique. There, one treats the constrained system as a free one, evolving with respect to the scalar field regarded as an internal time. The evolution is generated by a so-called evolution operator (further denoted as Θ). On the technical level the definiteness and uniqueness of the evolution reduces to the existence and the uniqueness of the self-adjoint extensions of Θ. In the previously investigated models this operator always admitted a unique extension [17,18], which ensured a unique evolution. The positive Λ however acts like a negative unbounded potential, thus one cannot immediately expect the same answer for the models with $\Lambda > 0$. Here we analyze in detail the self-adjointness of Θ, showing in particular that, for $\Lambda < \Lambda_c$, where Λ_c is a certain critical value (of the Planck order) it in fact admits a family of extensions. This property is crucial for further studies of the universe dynamics [19].

The paper is organized as follows. In Sec. II we briefly recall the basic features of the model and introduce the elements relevant for our investigation. Next, in Sec. III we determine the number of self-adjoint extensions of Θ corresponding to, respectively, the *subcritical* ($0 < \Lambda < \Lambda_c$, Sec. III A) and *supercritical* ($\Lambda \geq \Lambda_c$, Sec. III B) value of Λ, by probing the dimensionality of the deficiency spaces of Θ [20] via the method presented in [21] (Sec. IV). The properties of the physical Hilbert spaces built of the spectral decomposition of Θ are briefly analyzed for both the subcritical and supercritical case in Secs. IV and V. The article is concluded with Sec. VI, where the results are summarized and their physical consequences as well as the direct extensions are briefly discussed.

II. THE MODEL

Here we consider a model of a flat isotropic universe with positive cosmological constant $\Lambda > 0$ and a free scalar field as a matter content (see Appendix A in [10]). Its classical and kinematical description (in a loop quantization) is a direct analogy of the one used for the model with $\Lambda < 0$ [15].

The considered spacetime admits a foliation (parametrized by a time t) by isotropic 3-surfaces Σ and the metric

$$g = -N^2 dt^2 + a^2(t)^o q, \qquad (2.1)$$

where ${}^o q$ is a unit (fiducial) Cartesian metric on the surface Σ, N is a lapse function, and $a(t)$ is a scale factor. To describe the spacetime we use the canonical formalism, first selecting the fiducial triad ${}^o e^a_i$ orthonormal with respect to ${}^o q$ (and the cotriad ${}^o \omega^i_a$ dual to it), next introducing

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the canonical Ashtekar variables: connections A^i_a and triads E^a_i, which upon partial fixing of the gauge freedom can be represented just by a pair of canonically conjugated variables: the connection c and triad p coefficients,

$$A^i_a = cV_o^{-(1/3)}{}^o\omega^i_a, \qquad E^a_i = pV_o^{-(2/3)}\sqrt{{}^oq}\,{}^oe^a_i, \tag{2.2}$$

where V_o is the fiducial (with respect to ${}^oq$) volume of a certain comoving cubical region $\mathcal{V}$ introduced to regulate the divergences of the action and the Hamiltonian. The coefficients c and p are global degrees of freedom.

Our system is a constrained one, with the diffeomorphism and Gauss constraints automatically satisfied by a gauge choice. The only nontrivial constraint is a Hamiltonian one:

$$C = N(C_{\mathrm{gr}} + C_\phi), \tag{2.3a}$$

$$C_{\mathrm{gr}} = -\frac{1}{\gamma^2}\int_{\mathcal{V}} d^3x(\varepsilon_{ijk}e^{-1}E^{ai}E^{bj}F^k_{ab} - \gamma^2\Lambda), \tag{2.3b}$$

$$C_\phi = 8\pi G p^{-(3/2)}p_\phi^2, \tag{2.3c}$$

where $e := \sqrt{|\det E|}$, F^k_{ab} is the curvature of A^i_a: $F^k_{ab} := 2\partial_a A^k_b + \varepsilon^k_{ij}A^i_aA^j_b$, γ is the Barbero-Immirzi parameter, and p_ϕ is the canonical momentum of the scalar field ϕ.

The quantization process is a direct application of the methods of LQG, following in particular the Dirac program consisting of the following steps: (i) The system is first quantized on the kinematical level, with the constraint ignored. (ii) Next the constraint is promoted to a quantum operator $\hat{C}$ defined in some domain of the kinematical Hilbert space $\mathcal{H}^{\mathrm{kin}}$ identified in the previous step, and (iii) the physical Hilbert space $\mathcal{H}^{\mathrm{phy}}$ is built out of the states annihilated by it. Finally, (iv) the evolution picture is provided by selecting an internal time (in our case this role is played by ϕ) and defining the family of observables parametrized by it. In a slightly weaker sense, the evolution is defined by the unitary mapping between the spaces of "initial data." In the cases considered here it corresponds to a map:

$$\mathbb{R} \ni \phi \mapsto \Psi(\cdot, \phi) \in \mathcal{H}^{\mathrm{kin}}, \qquad \Psi \in \mathcal{H}^{\mathrm{phy}}. \tag{2.4}$$

Our goal here is the verification of the existence and uniqueness of such mapping.

The particular realization and the results of each of these steps is the following:

(i) To assess the geometry degrees of freedom we construct the analog of an LQG holonomy-flux algebra consisting of the holonomies along the straight lines and fluxes along the unit square surfaces, then proceed with the quantization method used for LQG. The resulting kinematical gravitational Hilbert space is

$$\mathcal{H}^{\mathrm{gr}} = L^2(\bar{\mathbb{R}}, d\mu_{\mathrm{Bohr}}), \tag{2.5}$$

where $\bar{\mathbb{R}}$ is a Bohr compactification of the real line. The basic operators are holonomies $\hat{h}^{(\lambda)}$ and unit fluxes (or "triads") $\hat{p}$. A particularly convenient basis of $\mathcal{H}^{\mathrm{gr}}$ consists of the eigenstates of $\hat{p}$ labeled by $v \in \mathbb{R}$ as follows:

$$\hat{p}|v\rangle = (2\pi\gamma\ell^2_{\mathrm{Pl}}\sqrt{\Delta})^{2/3}\mathrm{sgn}(v)|v|^{2/3}|v\rangle, \tag{2.6}$$

where Δ is the LQC *area gap* [22]. In this basis the scalar product is given by

$$\langle\psi|\psi'\rangle = \sum_{v\in\mathbb{R}}\bar{\psi}(v)\psi'(v). \tag{2.7}$$

The matter degrees of freedom are quantized via standard methods of quantum mechanics. In particular, the basic operators are the field $\hat{\phi}$ and its momentum $\hat{p}_\phi$ and the matter Hilbert space is spanned by the eigenstates of $\hat{\phi}$. The complete $\mathcal{H}^{\mathrm{kin}}$ has thus the form

$$\mathcal{H}^{\mathrm{kin}} = \mathcal{H}^{\mathrm{gr}} \otimes \mathcal{H}^\phi, \qquad \mathcal{H}^\phi = L^2(\mathbb{R}, d\phi). \tag{2.8}$$

(ii) The constraint (2.3) is first reexpressed in terms of holonomies and fluxes which are next promoted to operators. At present there are several prescriptions existing in the literature, which differ in the technical details: choice of the lapse, factor ordering, and symmetrization of an operator. In this paper we study three of them introduced in [10,11,24] and denoted, respectively, by APS, sLQC, and MMO prescriptions (specified in the points below). In all of these cases the quantum constraint can be brought to the form

$$\mathbb{1} \otimes \partial^2_\phi + \Theta_\Lambda \otimes \mathbb{1}, \qquad \Theta_\Lambda := \Theta_o - \Lambda V(v), \tag{2.9}$$

where an action of the operator Θ_o equals

$$-[\Theta_o\psi](v) = f_+(v)\psi(v-4) - f_o(v)\psi(v) + f_-(v)\psi(v+4), \tag{2.10}$$

with the form of $f_{o,\pm}$ depending on the particular prescription used and given respectively by

(i) APS:

$$f_\pm(v) = [B(v\pm 4)]^{-(1/2)}\tilde{f}(v\pm 2)[B(v)]^{-(1/2)}, \tag{2.11a}$$

$$f_o(v) = [B(v)]^{-1}[f_+(v) + f_-(v)], \tag{2.11b}$$

$$V(v) = \pi G\gamma^2\Delta\frac{|v|}{B(v)}, \tag{2.11c}$$

where [25]

$$\tilde{f}(v) = (3\pi G/8)|v|||v+1| - |v-1||, \quad (2.12a)$$
$$B(v) = (27/8)|v|||v+1|^{1/3} - |v-1|^{1/3}|^3 \quad (2.12b)$$

(ii) sLQC:

$$f_\pm(v) = \frac{3\pi G}{4}\sqrt{v(v\pm 4)}(v \pm 2), \quad (2.13a)$$
$$f_o(v) = 3\pi G v^2/2, \quad (2.13b)$$
$$V(v) = \pi G \gamma^2 \Delta v^2. \quad (2.13c)$$

(iii) MMO:

$$\begin{aligned} f_\pm(v) &= C g(v\pm 4) s_\pm(v\pm 2) \\ &\quad \times g^2(v\pm 2) s_\pm(v) g(v), \\ f_o(v) &= C g^2(v)[g^2(v-2)s_-^2(v) \\ &\quad + g^2(v+2)s_+^2(v)], \\ V(v) &= \frac{8\pi G\gamma^2\Delta}{27}\frac{g^6(v)}{|v|}, \end{aligned} \quad (2.14)$$

where

$$g(v) = ||1+1/v|^{1/3} - |1-1/v|^{1/3}|^{-1/2}, \quad (2.15a)$$
$$s_\pm(v) = \mathrm{sgn}(v\pm 2) + \mathrm{sgn}(v), \quad (2.15b)$$
$$C = \pi G/12. \quad (2.15c)$$

In all listed prescriptions the operators Θ_o and Θ_Λ are well defined in particular for $\varepsilon = 0$ (see the detailed discussion in [26] for APS and [24] for MMO).

At this point it is worth noting that for all the above cases the operator Θ_o is of the general form

$$\Theta_o = -b(v)(\hat{h}^{+2} - \hat{h}^{-2})a(v)(\hat{h}^{+2} - \hat{h}^{-2})b(v), \quad (2.16)$$

where $\hat{h}^\lambda|v\rangle = |v+\lambda\rangle$ and for large v the product [27]

$$a(v)b^2(v) = (3\pi G/4)v^2 + \mathrm{const} + o(1). \quad (2.17)$$

In fact, all the symmetric orderings considered so far in LQC literature (see [16,18] for examples) preserve the form (2.16) and correspond just to different distribution of v dependence between the functions a and b while preserving the property (2.17). This implies that between the orderings (and regularizations) of that class the coefficients $f_{o,\pm}$ differ just by a function behaving asymptotically like const + $o(1)$. On the other hand, the term $V(v)$ in (2.9) is affected just by the choices of the regularization and for the different ones its exact form differs just by $o(1)$.

(iii) Given the constraint operator in the form (2.9), one can find the physical Hilbert space, for example, by the group averaging techniques [28]. For that, however, one needs to know the spectral decomposition of Θ_Λ, thus its self-adjoint extension(s).
Before going to this step let us note that the structure of Θ_Λ and (2.9) provides the natural division of the domain of v onto the subsets (the *lattices*)

$$\mathcal{L}_\varepsilon = \{\varepsilon + 4n; n \in \mathbb{Z}\}, \qquad \varepsilon \in [0, 4[\quad (2.18)$$

preserved by the action of Θ_Λ. This division is naturally transferred to the splitting of $\mathcal{H}^{\mathrm{phy}}$ onto superselection sectors. In consequence it is enough to fix a particular value of ε and work just with the restriction of the domain of Θ_Λ to functions supported on $\mathcal{L}_\varepsilon$ only.
Further restriction comes from the fact that the considered system does not admit parity violating interactions. In consequence, the triad orientation reflection $v \mapsto -v$, being a large gauge symmetry, provides another natural division onto superselection sectors, namely the spaces of symmetric and antisymmetric states. For the rest of this work we select the sector corresponding to symmetric states with $\varepsilon = 0$. The studies are however straightforward extendable to all other sectors, as we discuss at the end of each section. Our particular choice allows one to further restrict the support of the functions to $\mathcal{L}_\varepsilon^+ := \mathcal{L}_\varepsilon \cap \mathbb{R}^+$.

(iv) A way of finding the physical Hilbert space and defining an evolution alternative to group averaging [and for the form of the constraint (2.9), equivalent to it [29]] is a reinterpretation of the system as a free one evolving along the scalar field playing the role of an internal time. The similarity of (2.9) with the Klein-Gordon equation

$$[\partial_\phi^2 \Psi](v,\phi) = -[\Theta_\Lambda \Psi](v,\phi) \quad (2.19)$$

allows one to directly apply the standard quantum mechanical methods for solving it. Such structure, in particular, introduces yet another splitting onto superselection sectors corresponding to positive and negative energies out of which we select the positive sector. In consequence, we can immediately write down the evolution between the initial data states on the constancy surfaces of ϕ, belonging to the projection of $\mathcal{H}^{\mathrm{gr}}$ onto the space spanned by the positive part of the spectrum of Θ_Λ,

$$\begin{aligned} U_{\phi_o,\phi}&: P_{\Theta_\Lambda \geq 0}\mathcal{H}^{\mathrm{gr}} \to P_{\Theta_\Lambda\geq 0}\mathcal{H}^{\mathrm{gr}}, \\ [U_{\phi_o,\phi}\Psi](v,\phi) &= e^{i(\phi-\phi_o)\sqrt{\Theta_\Lambda}+}\Psi(v,\phi_o), \end{aligned} \quad (2.20)$$

where the operator $P_{\Theta_\Lambda \geq 0}$ is the projection onto the positive part of the spectrum and $\sqrt{\Theta_\Lambda}+$ is the square root of Θ_Λ on the space $P_{\Theta_\Lambda \geq 0}\mathcal{H}^{\rm gr}$. For the evolution to be well defined and unitary, however, the operator Θ_Λ needs to be self-adjoint. Thus, the problem of the definiteness of the evolution reduces to the question about the self-adjointness of Θ_Λ, which we will investigate in the next section.

III. EXTENSIONS OF THE EVOLUTION OPERATOR

To start with, we note that the operator Θ_Λ defined via (2.9) and (2.19) is symmetric on the domain $\mathcal{D}$ of the finite linear combinations of eigenstates $|v\rangle$ of $\hat{p}$, a set which is itself dense in $\mathcal{H}^{\rm gr}$. To check whether Θ_Λ is furthermore essentially self-adjoint, we follow the method specified in [20,21], finding its deficiency indexes.

The first step is the identification of the deficiency subspaces $\mathcal{U}^\pm$ defined as the spaces of (kinematically) normalizable solutions $\psi^\pm$ to the equation

$$[\Theta_\Lambda \psi^\pm](v) = \pm i \psi^\pm(v). \qquad (3.1)$$

The dimensions of $\mathcal{U}^\pm$ are exactly the deficiency indexes needed to verify the self-adjointness. By inspecting the form of Θ_Λ provided in (2.9), (2.10), (2.11), (2.12), (2.13), (2.14), and (2.15) and taking into account the symmetry, we note that any solution $\psi^\pm$ to (3.1) is uniquely determined via its value $\psi^\pm(v=4)$. The spaces $\mathcal{U}^\pm$ are thus at most one-dimensional and nontrivial only when the solutions are normalizable.

To verify this property of $\psi^\pm$ we first analyze their asymptotes. To start with, we rewrite the equation (3.1), being the 2nd order difference equation, in a 1st order form, introducing

$$\vec{\psi}^{\,\pm}(v) := \begin{pmatrix} \psi^\pm(v) \\ \psi^\pm(v-4) \end{pmatrix}. \qquad (3.2)$$

In this notation the considered equation takes the form

$$\vec{\psi}^{\,\pm}(v+4) = \boldsymbol{A}(v)\vec{\psi}^{\,\pm}(v), \qquad (3.3)$$

where, applying the notation introduced in Eqs. (2.9) and (2.10), one can write the matrix $\boldsymbol{A}$ as

$$\boldsymbol{A}(v) = \begin{pmatrix} \frac{f_o(v) - \Lambda V(v) \mp i}{f_+(v)} & -\frac{f_-(v)}{f_+(v)} \\ 1 & 0 \end{pmatrix}. \qquad (3.4)$$

The next step is expressing $\vec{\psi}^{\,\pm}$ as a linear combination of the appropriately selected asymptotic functions (further denoted as $\underline{\psi}_\Lambda^\pm$) and rewriting (3.3) as the equation for the coefficients of that combination. At this point we note that the preliminary numerical inspection shows qualitatively different asymptotic behavior of $\psi^\pm$ depending on whether the value of Λ is below or above certain (found analytically [31]) critical value Λ_c related to the critical energy density ρ_c [10] or the area gap Δ as follows:

$$\Lambda_c := 8\pi G \rho_c = 3/(\gamma^2 \Delta). \qquad (3.5)$$

In consequence, the more detailed analytical treatment requires considering these two cases separately. Since the energy density operator has been shown to be bounded by ρ_c [11,26] and the cosmological constant carries a residual gravitational energy, it is natural from the physical point of view to restrict the consideration just to $\Lambda < \Lambda_c$, although for completeness we will also dedicate some attention to the $\Lambda \geq \Lambda_c$ case.

A. Subcritical Λ

In this case, as asymptotic functions we select $\underline{\psi}_\Lambda^\pm$ defined as

$$\underline{\psi}_\Lambda^\pm := |v|^{-1} e^{\pm i \omega(\Lambda)|v|}, \qquad (3.6)$$

where $\omega(\Lambda) \in]0, \pi/4[$ equals [32]

$$\omega(\Lambda) = \frac{1}{2}\arccos\left[\sqrt{\frac{\gamma^2\Delta\Lambda}{3}}\right] = \frac{1}{2}\arccos\left[\sqrt{\frac{\Lambda}{\Lambda_c}}\right]. \qquad (3.7)$$

With that choice we define the vector of coefficients for each pair of consecutive points on $\mathcal{L}_0^+$,

$$\vec{\psi}^{\,\pm}(v) = \boldsymbol{B}(v-4)\vec{\chi}^{\,\pm}(v), \qquad (3.8)$$

where the transformation matrix $\boldsymbol{B}$ is defined as

$$\boldsymbol{B}(v) := \begin{pmatrix} \underline{\psi}_\Lambda^+(v+4) & \underline{\psi}_\Lambda^-(v+4) \\ \underline{\psi}_\Lambda^+(v) & \underline{\psi}_\Lambda^-(v) \end{pmatrix}. \qquad (3.9)$$

Having that, we can rewrite the equation (3.3) as follows:

$$\begin{aligned} \vec{\chi}^{\,\pm}(v+4) &= \boldsymbol{B}^{-1}(v)\boldsymbol{A}(v)\boldsymbol{B}(v-4)\vec{\chi}^{\,\pm}(v) \\ &:= \boldsymbol{M}(v)\vec{\chi}^{\,\pm}(v). \end{aligned} \qquad (3.10)$$

The exact coefficients of the matrix $\boldsymbol{M}(v)$ can be calculated explicitly. The property relevant for us is that for each of the prescriptions listed in Sec. II it features the following asymptotic behavior (identified via calculating the series expansion):

$$\boldsymbol{M}(v) = \mathbb{1} + \boldsymbol{O}(v^{-2}), \qquad (3.11)$$

where $\boldsymbol{O}(v^{-n})$ denotes a matrix, whose coefficients asymptotically behave like $O(v^{-n})$. This implies immediately (see Sec. 4 of [21]) the existence of the limit

$$\lim_{n\to\infty} \vec{\chi}^{\,\pm}(4n) =: \vec{\chi}^{\,\pm}, \qquad (3.12)$$

such that

$$\vec{\chi}^{\,\pm}(v) = \vec{\chi}^{\,\pm} + \vec{O}(v^{-1}). \qquad (3.13)$$

In consequence,

$$\psi^\pm(v) = (\underline{\psi}_\Lambda^+(v), \underline{\psi}_\Lambda^-(v)) \cdot \vec{\chi}^{\,\pm} + O(v^{-2}). \qquad (3.14)$$

This, together with the fact that $\psi^\pm$ is well defined and finite everywhere, implies that their norm with respect to the inner product (2.7) is finite.

Combining the above observation with the structure of eigenspaces discussed earlier, we conclude that the deficiency spaces $\mathcal{U}^\pm$ are both one-dimensional. Therefore [20,21] the operator Θ_Λ *is not* essentially self-adjoint, although it *admits a family* of self-adjoint extensions. Each extension corresponds to the unitary transformation

$$U\colon \mathcal{U}^+ \to \mathcal{U}^-. \tag{3.15}$$

Since $\mathcal{U}^\pm$ are one-dimensional, the only possible transformations which map the normalized ψ^+ into the space $\mathcal{U}^-$ are as follows:

$$\psi^+ \mapsto U^\alpha \psi^+ = e^{i\alpha}\psi^-, \tag{3.16}$$

where ψ^- is also assumed to be normalized. The family of possible extensions is thus labeled by one parameter $\alpha \in [0, 2\pi]$.

The above result can be extended in a straightforward way to other superselection sectors labeled by ε. The particular form of the extension and the details of its result depend on the prescription used. For the MMO one, since the triad orientations (positive and negative v) separate (see the detailed discussion in [8,24]), one can always restrict the consideration to $v > 0$. In consequence, the space of solutions to (3.1) is again one-dimensional and the deficiency functions are uniquely determined by their value at $v = \varepsilon$. Thus, the analysis of the asymptotics described above can be applied in this case without any modifications providing exactly the same result as for $\varepsilon = 0$.

For the remaining two prescriptions, the situation is slightly more complicated. Namely, for generic ε the eigenspaces of Θ_Λ corresponding to any eigenvalue, including $\pm i$, are two-dimensional. Also to verify their normalizability, one needs to check the asymptotics independently for positive and negative v. Nonetheless it can still be done by direct application of the method used for $\varepsilon = 0$ to each of the limits. The result is the same, although while analogs of (3.12) are still well defined (and the rate of convergence is the same), generically

$$\lim_{n\to\infty} \vec{\chi}(\varepsilon + 4n) \neq \lim_{n\to\infty} \vec{\chi}(\varepsilon - 4n). \tag{3.17}$$

As for $\varepsilon = 0$ all the solutions to (3.1) are normalizable. Now however $\dim(\mathcal{U}^+) = \dim(\mathcal{U}^-) = 2$, so the self-adjoint extensions of Θ_Λ are now labeled by the elements of the $U(2)$ group.

Restricting the studies to the symmetric functions does not change the result for $\varepsilon \neq 2$ as the parity reflection maps the lattice $\mathcal{L}_\varepsilon$ onto $\mathcal{L}_{4-\varepsilon}$, disjoint from the original one. In the only exceptional case $\varepsilon = 2$, the symmetry imposes an additional constraint between the values of the eigenfunctions at $v = 2$ and $v = -2$. In consequence, the eigenspaces are again one-dimensional and the results are exactly the same as for $\varepsilon = 0$.

At this point it is also worth noting that the modifications to the evolution operator introduced by different choices of ordering of the (quite general) class discussed at the end of point (ii) of Sec. II do not affect the asymptotic properties of $\boldsymbol{M}$ (3.10), that is (3.11) remains true. In consequence, the above results extend also to these more general situations.

B. Supercritical Λ

In the case $\Lambda \geq \Lambda_c$, it is convenient to introduce the following change of representation for a general superselection sector ε:

$$\psi(v) \mapsto \tilde{\psi}(v) = (-1)^{(v-\varepsilon)/4}\psi(v). \tag{3.18}$$

It is trivial to note that the kinematical inner product (2.7) between transformed functions is given by a formula identical to (2.7). On the other hand, the examination of the form of Θ_Λ provided by (2.9), (2.10), (2.11), (2.12), (2.13), (2.14), and (2.15) shows that it transforms into

$$\Theta_\Lambda \to \tilde{\Theta}_\Lambda = -\Theta_{\Lambda_c - \Lambda} + A(v)\mathbb{1}, \tag{3.19}$$

where $A(v)$ is always finite and decays as $O(v^{-2})$, thus $A(v)1$ is a compact operator. This feature allows immediately to apply Kato's perturbation theory [33] and the self-adjointness of Θ_Λ for $\Lambda \leq 0$ [18] to conclude that for $\Lambda \geq \Lambda_c$ the operator Θ_Λ is also essentially self-adjoint.

IV. THE SPECTRAL PROPERTIES FOR $\Lambda < \Lambda_c$

For subcritical values of Λ, we have shown in Sec. III A that the evolution operator Θ_Λ admits (in the principal case $\varepsilon = 0$ considered here) a one-parameter family of extensions Θ_α. Each of these extensions defines an evolution via (2.20) with Θ_Λ replaced by Θ_α. In order to identify the physical Hilbert space $\mathcal{H}^{\rm phy}_\alpha$ corresponding to each extension, we need to know (the positive part of) the spectrum of Θ_α. Here we analyze some properties of it, as well as the eigenspaces corresponding to its elements.

Let us start with the eigenfunctions. By inspection one can easily notice that the analysis of the asymptotics of the deficiency functions performed in Sec. III extends directly to any eigenfunction corresponding to any complex eigenvalue, with the same form of the asymptotic functions (3.6) and convergence rates (3.13). In consequence, every eigenfunction of Θ_Λ is explicitly normalizable, being thus an element of $\mathcal{H}^{\rm gr}$. This in turn implies that the spectrum of each Θ_α is purely discrete.

To identify the spectra $\mathrm{Sp}(\Theta_\alpha)$, we first determine the domain of each extension, applying the theorem X.2 of [20]. It follows from it that the domain $\mathcal{D}_\alpha$ of Θ_α in our case equals

$$\mathcal{D}_\alpha = \{\psi + \psi^+ + U^\alpha\psi^+;\ \psi \in \mathcal{D},\ \psi^\pm \in \mathcal{U}^\pm\}, \tag{4.1}$$

where U^α is given by (3.16). On the other hand, $\mathcal{D}_\alpha$ is spanned by those of the (normalized) eigenfunctions $e_\omega(v)$ whose eigenvalues $\omega \in \mathrm{Sp}(\Theta_\alpha)$. As the eigenfunctions are normalizable, the ones selected by that condition also belong to $\mathcal{D}_\alpha$. Since the original domain $\mathcal{D}$ of Θ_Λ is (a Cauchy completion with respect to the graph norm of) a space of finite linear combinations of $|v\rangle$, only the term $\psi^+ + U^\alpha\psi^+$ contributes to the asymptotics of the elements $\mathcal{D}_\alpha$. In consequence, $\mathcal{D}_\alpha$ is spanned by (all and only) the eigenfunctions e_ω which converge to a combination $\psi^+ + U^\alpha\psi^+$ for some $\psi^+ \in \mathcal{U}^+$.

The above selection criterion, although precise, is not convenient for practical purposes. To bring it to a simpler form, we remind that all the eigenfunctions, including the deficiency functions and e_ω, converge to linear combinations of $\underline{\psi}^\pm_\Lambda$. Furthermore, as Θ_Λ is a real operator, the limit of e_ω is necessarily of the form

$$e_\omega(v) = \lambda(\omega)[e^{i\beta(\omega)}\underline{\psi}^+_\Lambda(v) + e^{-i\beta(\omega)}\underline{\psi}^-_\Lambda(v)] + O(v^{-2}), \tag{4.2}$$

where $\lambda(\omega) \in \mathbb{C}$ and the phase shifts $\beta(\omega) \in [0, 2\pi]$. Obviously the term $\psi^+ + U^\alpha\psi^-$ has the same form of the limit, up to an additional rotation by a global phase. Furthermore, the transformation $\beta \to \beta \pm \pi$ corresponds just to change of sign. In consequence, there is a one to one correspondence between the parameters α and $\beta \in [0, \pi[$ which thus uniquely label the extensions.

As one needs just to compare the asymptotic behavior of the eigenfunction against the functions of a very simple analytic form, the classification with respect to β is much better suited for practical applications, like e.g. the explicit identification of the spectra of the extended operators, as well as for finding the bases of the physical Hilbert spaces. One has to remember, however, that this classification is just a more convenient form of the previous one, not an alternative to it.

The above results, derived for the superselection sector $\varepsilon = 0$, generalize easily to other sectors, although the exact results depend (as in the studies of Sec. III A) on the particular prescription. Namely, for the MMO prescription, due to nondegeneracy of the eigenspaces of Θ_Λ, the analysis presented in this section can be repeated exactly, giving exactly the same results. For the remaining two prescriptions, one has to introduce slight modifications taking into account the twofold degeneracy of the eigenvalues. In particular, the label of the extension inherited from the label of the unitary transformation U (3.15) via (4.1) is now an element of the $U(2)$ group. All the eigenfunctions of Θ_Λ are however again explicitly normalizable, and the ones spanning a particular extension are selected by the condition that a given eigenfunction e_ω belongs to $\mathcal{D}_\alpha$ iff there exists $\psi^+ \in \mathcal{U}^+$ such that the considered eigenfunction converges to a combination $\psi^+ + U^\alpha\psi^+$, where U^α is a transformation (3.15) corresponding to a particular value of the label $\alpha \in U(2)$.

V. PHYSICAL HILBERT SPACE FOR $\Lambda \geq \Lambda_c$

For these cases we have proved in Sec. III B that the operator Θ_Λ is essentially self-adjoint. Also the form (3.19) of Θ_Λ after the representation change (3.18) suggests that qualitatively its spectrum should resemble $\mathrm{Sp}(\Theta_{\Lambda'})$, where $\Lambda' = \Lambda_c - \Lambda \leq 0$. Thus, we expect the whole spectrum to be quite rich. In particular, the essential part of it equals just $\mathrm{Sp}_{\mathrm{es}}(-\Theta_{\Lambda'})$. As $\mathrm{Sp}_{\mathrm{es}}(\Theta_{\Lambda'})$ equals either $\mathbb{R}^+$ (for $\Lambda' = 0$) or is empty ($\Lambda' < 0$) [18] $\mathrm{Sp}_{\mathrm{es}}(\Theta_\Lambda)$ is purely nonpositive. On the other hand, since only $P_{\Theta_\Lambda > 0}\mathcal{H}^{\mathrm{gr}}$ enters (2.20), only the positive part of $\mathrm{Sp}(\Theta_\Lambda)$ is relevant from the physical point of view. From the above reasoning it follows immediately that it has to be purely discrete [34]. In this section we will study exactly this part. The analysis will be again restricted just to the superselection $\varepsilon = 0$ and the symmetric functions.

The discreteness of the positive part of the spectrum implies that the eigenfunctions corresponding to it have to be explicitly normalizable. One can show, however, that no such function exists at least for selected prescriptions and superselection sector. Indeed, from (2.9) and (2.10) and the positivity of $f_{o,\pm}(v)$ and $\Lambda_c V(v) - f_o(v)$ for $v \geq 4$ follows that the solution to the equation $\Theta_\Lambda \psi_{\omega,\Lambda} = \omega^2 \psi_{\omega,\Lambda}$ satisfies the relation

$$\begin{aligned} |\psi_{\omega,\Lambda}(v+4)| &\geq \frac{\Lambda V(v) - f_o(v) + \omega^2}{f_+(v)}|\psi_{\omega,\Lambda}(v)| \\ &\quad - \frac{f_-(v)}{f_+(v)}|\psi_{\omega,\Lambda}(v-4)| \\ &\geq \frac{\Lambda_c V(v) - f_o(v)}{f_+(v)}|\psi_{\omega,\Lambda}(v)| \\ &\quad - \frac{f_-(v)}{f_+(v)}|\psi_{\omega,\Lambda}(v-4)|. \end{aligned} \tag{5.1}$$

This and the fact that for the chosen superselection sector all the eigenfunctions ψ_ω are determined by their initial values $\psi_\omega(v = 4)$ implies

$$|\psi_{\omega,\Lambda}(4)| = |\psi_{0,\Lambda_c}(4)| \Rightarrow |\psi_{\omega,\Lambda}(8)| \geq |\psi_{0,\Lambda_c}(8)|, \tag{5.2}$$

thus, defining the ratios

$$\chi_{\omega,\Lambda}(v) := -\psi_{\omega,\Lambda}(v)/\psi_{\omega,\Lambda}(v-4), \tag{5.3}$$

we have

$$\chi_{\omega,\Lambda}(8) \geq \chi_{0,\Lambda_c}(8). \tag{5.4}$$

Furthermore, $\chi_{\omega,\Lambda}$ satisfy the equation [following directly from (2.9) and (2.10)]

$$\chi_{\omega,\Lambda}(v+4) = \frac{\Lambda V(v) - f_o(v) + \omega^2}{f_+(v)} - \frac{f_-(v)}{f_+(v)}\frac{1}{\chi_{\omega,\Lambda}(v)}, \tag{5.5}$$

which together with [following from (2.11), (2.12), (2.13), (2.14), and (2.15)] positivity of $f_\pm(v)$ and $\Lambda_c V(v) - f_o(v)$

for $v \geq 4$ implies

$$\forall\ v \geq 8:\ \chi_{\omega,\Lambda}(v) \geq \chi_{0,\Lambda_c}(v) \Rightarrow \chi_{\omega,\Lambda}(v+4) \geq \chi_{0,\Lambda_c}(v+4). \tag{5.6}$$

In consequence, by induction we have

$$|\psi_{\omega,\Lambda}(4)| \geq |\psi_{0,\Lambda_c}(4)| \Rightarrow \forall\ n \in \mathbb{Z}^+ : |\psi_{\omega,\Lambda}(4n)| \geq |\psi_{0,\Lambda_c}(4n)|. \tag{5.7}$$

On the other hand, taking as $\underline{\psi}^{\pm}(v)$ the functions

$$\underline{\psi}^{+}(v) = \frac{(-1)^{v/4}}{\sqrt{|v|}}, \qquad \underline{\psi}^{-}(v) = \frac{(-1)^{v/4}}{\sqrt{|v|}} \ln|v|, \tag{5.8}$$

one can perform the analysis of the asymptotics analogous to the one in Sec. III A, showing that

$$\psi_{0,\Lambda_c}(v) = \frac{(-1)^{v/4}}{\sqrt{|v|}}(c_1 + c_2 \ln|v|) + O(v^{-3/2}\ln(v)), \tag{5.9}$$

where, due to the existence of both $\prod_{n=n_0}^{\infty} M(4n)$ and $\prod_{n=\infty}^{n_0} M(4n)^{-1}$ [where M is an analog of the matrix defined in (3.10)] for some large enough n_0, and the fact that the eigenfunction is uniquely determined by its value at $v = 4$, at least one of the coefficients c_1, c_2 does not vanish.

From the relations (5.7) and (5.9) we see that for $\Lambda \geq \Lambda_c$ none of the eigenfunctions corresponding to the positive eigenvalues are normalizable. In consequence, the positive part of the spectrum of Θ_Λ is empty, thus the physical Hilbert spaces corresponding to those values of Λ are trivial.

This result cannot be immediately extended to the remaining superselection sectors as for some prescriptions and values of ε the validity of the inequalities (5.1) and (5.2) (generalized to include the initial data at two points) as well as the statement of nonvanishing of $|c_1| + |c_2|$ might be affected near $v = 0$ by the different behavior of the functions $f_\pm$, f_o, B there. Therefore we cannot exclude the existence of the normalizable eigenfunction in those cases. One can see however that, as up to the transformation (3.18), the eigenfunctions have the same asymptotic properties as the (corresponding to the negative eigenvalues) eigenfunctions of Θ_Λ for $\Lambda \leq 0$. In consequence, all the normalizable eigenfunctions have to decay exponentially ($\Lambda > \Lambda_c$) or like $O(v^{-3/2}\ln(v))$ ($\Lambda = \Lambda_c$). Furthermore, due to the form of coefficients of Θ_Λ (2.10) they have to enter this behavior already at $|v| \approx 4$. This is possible only for low values of ω as for the larger ones the term ω^2 is a dominating one at $|v| \leq 4$, which again forces the behavior similar to the asymptotic one. In consequence, any possible normalizable eigenfunctions necessarily correspond to small eigenvalues and are peaked near the classical singularity.

VI. CONCLUSIONS

We have considered the evolution operator Θ_Λ defining the evolution of the isotropic flat universe with massless scalar field and positive cosmological constant quantized within the framework of loop quantum cosmology. For the investigation three exact forms of the operator corresponding to particular prescriptions [10] (APS), [11] (sLQC), and [24] (MMO) were selected. Our main goal was the verification of its self-adjointness as the condition necessary to generate a unique unitary evolution in the Schrödinger picture. We also investigated the properties of the Hilbert spaces defined by the spectra of possible self-adjoint extensions of Θ_Λ. All the results were derived analytically, without resorting to the numerical methods.

The results of the studies happen to depend on the value of the cosmological constant Λ. Namely, one can divide the set of its values onto two regions separated by the critical value related with the critical energy density [10] via the equality $\Lambda_c = 8\pi G\rho_c$ for which the properties of Θ_Λ are qualitatively different.

For $0 < \Lambda < \Lambda_c$ (denoted as subcritical) Θ_Λ admits many self-adjoint extensions, each of them defining inequivalent (at least at the mathematical level) unitary evolution. The extensions are labeled by the elements of the $U(1)$ or $U(2)$ group, depending on the superselection sector. In particular, once the studies are restricted to the symmetric functions only, the groups of labels G are

$$G = \begin{cases} U(1), & \text{MMO}, \\ U(2), & \text{APS and sLQC}, \ \varepsilon \neq 0, 2, \\ U(1), & \text{APS and sLQC}, \ \varepsilon = 0, 2. \end{cases} \tag{6.1}$$

Once the self-adjoint extensions were identified their spectral properties were also studied. It was shown that the spectrum of each extension is discrete, thus the physical Hilbert space spanned by the set of normalizable eigenfunctions of Θ_Λ.

Although the primary objective of investigation was three particular forms of the evolution operator following from particular choices of factor ordering and regularization, the above results generalize immediately to a quite general class of orderings, namely the ones for which Θ_o takes the form specified by (2.16) and (2.17).

For $\Lambda \geq \Lambda_c$ (supercritical) we found the relation with the operators Θ_Λ for $\Lambda \leq 0$, which allowed one to show that the evolution operator is essentially self-adjoint, thus generating a unique unitary evolution. Further studies have shown however that for the superselection sector $\varepsilon = 0$ the positive part of the spectrum of Θ_Λ is empty, thus the physical Hilbert space defined by it is trivial. This situation might change in other superselection sectors. There however, even if nontrivial, the Hilbert space does not admit any physically interesting states. Also the generalization to other factor orderings and regularizations of Θ_Λ is not straightforward as it is not obvious that the relation

(3.19) will hold [with $A(v)\mathbb{1}$ being of the trace class] for every choice admitted by the form (2.16) of Θ_o.

The result of the above paragraph is analogous to the properties of the scalar field energy density operator performed in [26], where it was shown that for $\Lambda \geq \Lambda_c$ the absolutely continuous part of the spectrum of that operator is entirely nonpositive and the eigenfunctions corresponding to the positive elements of the spectrum (necessarily belonging to its discrete part) are peaked about $v = 0$.

In the subcritical case $\Lambda < \Lambda_c$ the existence of nonunique extensions implies, in particular, that the quantum evolution of the system is not explicitly unique. However, the detailed studies of its dynamics show [19] that in the semiclassical regime the dynamical predictions are surprisingly unique and in the limit $v \rightarrow \infty$ consistent with the (unique) analytic extension of the classical trajectory.

To conclude, let us note that the results regarding self-adjointness directly extend (with the exception of the case $\Lambda = \Lambda_c$) to the cases of different topologies ($K = \pm 1$), as the terms in Θ_Λ present in such models are subleading with respect to the term $\Lambda V(v)$. Furthermore applying the methods presented here, one can easily show that for the models $\Lambda = 0$ and $K = -1$ (defined in [13]) the evolution operator also admits nonunique extensions. By the relation (3.19) this result applies also to $\Lambda = \Lambda_c$, $K = +1$. On the other hand, the same argument and [17] imply the self-adjointness for $\Lambda = \Lambda_c$, $K = -1$.

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