

**Gravity quantized: Loop quantum gravity with a scalar field**Marcin Domagała,<sup>1,\*</sup> Kristina Giesel,<sup>2,3,†</sup> Wojciech Kamiński,<sup>1,‡</sup> and Jerzy Lewandowski<sup>1,4,§</sup><sup>1</sup>*Instytut Fizyki Teoretycznej, Uniwersytet Warszawski, ul. Hoża 69, 00-681 Warszawa (Warsaw), Polska (Poland)*<sup>2</sup>*Excellence Cluster Universe, Technische Universität München, Boltzmannstrasse 2, 85748 Garching, Germany*<sup>3</sup>*Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803, USA*<sup>4</sup>*Institute for Gravitation and the Cosmos, Physics Department, Penn State, University Park, Pennsylvania 16802, USA*

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...“but we do not have quantum gravity.” This phrase is often used when analysis of a physical problem enters the regime in which quantum gravity effects should be taken into account. In fact, there are several models of the gravitational field coupled to (scalar) fields for which the quantization procedure can be completed using loop quantum gravity techniques. The model we present in this paper consists of the gravitational field coupled to a scalar field. The result has similar structure to the loop quantum cosmology models, except that it involves all the local degrees of freedom of the gravitational field because no symmetry reduction has been performed at the classical level.

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**I. INTRODUCTION**

The recent advances in loop quantum gravity (LQG) [1–4] strongly suggest that the goal of constructing a candidate for quantum theory of gravity and the standard model is within reach. Remarkably, that goal can be addressed within the canonical formulation of the original Einstein’s general relativity in four-dimensional spacetime. A way to define “physical” dynamics in a background independent theory, where spacetime diffeomorphisms are treated as a gauge symmetry, is the framework of relational Dirac observables (often also called “partial” observables [5–8], Sec. I.2 of [2]). The main idea is that part of the fields adopt the role of a dynamically coupled observer, with respect to which the physics of the remaining degrees of freedom in the system is formulated. In this framework the emergence of the dynamics, time, and space can be explained as an effect of the relations between the fields. As far as technical issues of a corresponding quantum theory are concerned, the most powerful example of the relational observables framework is the deparametrization technique [9–12]. This allows one to map canonical general relativity into a theory with a (true) nonvanishing Hamiltonian that is independent of the (emergent) time provided by the observer fields. All this can be achieved at the classical level; the framework of LQG itself provides then the tools of the quantum theory like quantum states, the Hilbert spaces, quantum operators of the geometry and fields, and well-defined quantum operators for the classical constraints of general relativity (see [2,4], and references therein). The combination of LQG with the relational observables and deparametrization framework makes it possible to construct general relativistic quantum models. Applying LQG techniques to perform the

quantization step has the consequence that the quantum fields of the standard model have to be reintroduced within the scheme of LQG. This is due to the reason that the standard quantum field theory (QFT) defined on the Minkowski (or even anti-de Sitter) background is incompatible with the quantization approach used in LQG. Therefore, the resulting quantum theory of gravity cannot be just coupled to the standard model in its present form. The formulation of the full standard model within LQG will require some work. For this reason, we proceed step by step, increasing gradually the level of complexity. The first step was constructing various cosmological models by analogy with LQG by performing a symmetry reduction already at the classical level. They give rise to loop quantum cosmology (LQC) [13–19]. We have learned from them a lot about qualitative properties of quantum spacetime and its quantum dynamics [20,21]. That knowledge is very useful in performing the second step, which is introducing quantum models with the full set of the local gravitational degrees of freedom. The first quantum model of the full, four-dimensional theory of gravity was obtained by applying LQG techniques [22] to the Brown-Kuchar model of gravity coupled to dust [9]. In the current paper we apply LQG to the model introduced by Rovelli and Smolin [23] whose classical canonical structure was studied in detail by Kuchar and Romano [24]. This is a model of gravity coupled to a massless scalar field. Our goal is to complete the construction of the quantum model with the tools of LQG. In the first part of the paper (Secs. I and II) we introduce the model, study the structure of the space of solutions to the quantum constraints, and study the Dirac observables, assuming only suitable Hilbert products and operators exist. The result of this part is a list of mathematical elements necessary and sufficient for the model to exist. In the second part (Sec. III) we apply the framework of LQG. We show it provides the necessary Hilbert spaces and operators, and we complete the construction of the model.

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## II. CANONICAL GRAVITY COUPLED TO A CLASSICAL SCALAR FIELD

### A. The standard approach

The point of our interest in this paper is gravity coupled to a scalar field. We are considering a metric tensor field  $q_{ab}$  and a scalar field  $\phi$  on a 3-manifold  $M$  (the space). The conjugate momenta are denoted, respectively, by  $p^{ab}$  and  $\pi$ . The only nonvanishing Poisson brackets among them are

$$\begin{aligned} \{q_{ab}(x), p^{cd}(y)\} &= \delta(x, y) \delta_{(a}^c \delta_{b)}^d, \\ \{\phi(x), \pi(y)\} &= \delta(x, y). \end{aligned} \quad (2.1)$$

The intrinsic and extrinsic geometry of  $M$  (with  $M$  being the Cauchy surface of four-dimensional spacetime) is described by the first pair of canonically conjugate variables  $(q_{ab}, p^{ab})$ . The field  $q_{ab}$  defines the intrinsic Riemann geometry of  $M$ , whereas  $p^{ab}$  contains the information about the extrinsic curvature of  $M$  embedded in the spacetime.

The variables  $(q_{ab}, p^{ab})$  are known from the standard canonical formulation of gravity usually called Arnowitt-Deser-Misner (ADM) formalism [25] (see also Chapter 10 and Appendix E of [26]). But one can use any other variables in this part of our paper (Secs. I and II). In Sec. III we will apply LQG, and therein we will be using the Ashtekar-Barbero variables  $(A_a^i, P_i^a)$ ,  $i = 1, 2, 3$  (and the notation of [4]). They are also canonically conjugate to each other, and the only nonvanishing Poisson bracket is

$$\{A_a^i(x), P_j^b(y)\} = \delta(x, y) \delta_a^b \delta_j^i. \quad (2.2)$$

The intrinsic and extrinsic geometry of  $M$  can be recovered out of them, as they are defined by the orthonormal coframe  $e_a^i$ , the corresponding connection 1-form  $\Gamma_a^i$ , the extrinsic curvature 1-form  $K_a^i$ , and a fixed Barbero-Immirzi parameter  $\gamma$  (for its value see [27–29]), namely,

$$A_a^i = \Gamma_a^i + \gamma K_a^i, \quad P_i^a = \frac{1}{16\pi G \gamma} e_a^j e_b^k \eta^{abc} \epsilon_{ijk}, \quad (2.3)$$

where  $\eta^{123} = 1 = \epsilon_{123}$  and  $\eta^{abc}$ ,  $\epsilon_{abc}$  are completely antisymmetric.

The fields  $(A_a^i, P_i^a)$  set an  $\mathfrak{su}(2)$  valued 1-form and, respectively,  $\mathfrak{su}(2)^*$  valued vector density

$$A = A_a^i(x) \tau_i \otimes dx^a, \quad P = P_i^a(x) \tau^i \otimes \frac{\partial}{\partial x^a}, \quad (2.4)$$

where  $x^a$  are local coordinates in  $M$ ,  $\tau_1, \tau_2, \tau_3 \in \mathfrak{su}(2)$  is a basis such that

$$\eta(\tau_i, \tau_j) := -2 \text{Tr}(\tau_i \tau_j) = \delta_{ij},$$

and  $\tau^1, \tau^2, \tau^3$  is the dual basis.

Einstein's theory of gravity is subject to constraints. In the standard ADM approach we have two constraints, namely, the vector constraint generating the diffeomorphisms of  $M$

and the scalar constraint generating dynamics, that is, diffeomorphisms orthogonal to the Cauchy hypersurface  $M$ :

$$C_a(x) = C_a^{\text{gr}}(x) + \pi(x) \phi_{,a}(x), \quad (2.5)$$

$$\begin{aligned} C(x) &= C^{\text{gr}}(x) + \frac{1}{2} \frac{\pi^2(x)}{\sqrt{q(x)}} + \frac{1}{2} q^{ab}(x) \phi_{,a}(x) \phi_{,b}(x) \sqrt{q(x)} \\ &\quad + V(\phi) \sqrt{q(x)}, \end{aligned} \quad (2.6)$$

where the terms  $C_a^{\text{gr}}$  and  $C^{\text{gr}}$  involve the gravitational field variables  $q_{ab}$  and  $p^{ab}$  only.

In LQG, the fields  $q_{ab}$  and  $p^{ab}$  in the constraints are expressed by the variables  $A_a^i$  and  $P_i^a$ , and we get an additional constraint—the Gauss constraint generating the “Yang-Mills”<sup>1</sup> gauge transformations of the fields  $(A, P)$ :

$$G_a^i(x) = \partial_a P_i^a + \epsilon_{ij}{}^k A_a^j P_k^a. \quad (2.7)$$

All the transformations generated by the vector, the scalar, and the Yang-Mills constraint are gauge transformations, because the constraints are of first class.

In Secs. I and II the choice of the variables describing the gravitational part does not matter, so one can use either the ADM variables  $(q_{ab}, p^{ab})$  and the constraints (2.5) and (2.6) or, respectively, the Ashtekar-Barbero variables  $(A_a^i, P_i^a)$  and the constraints (2.5), (2.6), and (2.7). In Sec. III, the latter choice is necessary, because we will apply LQG. For the sake of the continuity, we will stick to the Ashtekar-Barbero variables, remembering that  $q_{ab}$ ,  $p^{ab}$ ,  $C^{\text{gr}}$ , and  $C_a^{\text{gr}}$  should be considered as functions of  $(A_a^i, P_i^a)$ .

Each choice of the fields  $(A_a^i, P_i^a, \phi, \pi)$  defines a point in the phase space  $\Gamma$ . The solutions to the constraints form a constraint surface. We will also consider separately the phase space of gravitational degrees of freedom denoted by  $\Gamma_{\text{gr}}$ , which by definition is set by the pairs  $(A_a^i, P_i^a)$ .

By assuming that the vector and the scalar constraints are satisfied

$$C(x) = 0, \quad C_a(x) = 0, \quad (2.8)$$

we can solve the vector constraint in (2.5) for the gradient  $\phi_{,a}$  obtaining  $\phi_{,a} = -\frac{C_a^{\text{gr}}}{\pi}$  and inserting this into the scalar constraint (2.6). What we get, remembering (2.8) and solving the scalar constraint for  $\pi$ , is an expression for  $\pi^2$  as a function of the geometry variables  $(A_a^i, P_i^a)$  and the potential  $V(\phi)$  only,

$$\begin{aligned} \pi^2 &= \sqrt{q}(-C^{\text{gr}} + \sqrt{q}V(\phi)) \\ &\quad \pm \sqrt{(C^{\text{gr}} + \sqrt{q}V(\phi))^2 - q^{ab} C_a^{\text{gr}} C_b^{\text{gr}}}. \end{aligned} \quad (2.9)$$

<sup>1</sup>Although we do not consider the Yang-Mills theory itself, the Ashtekar-Barbero variables are subject to the gauge transformations known from the Yang-Mills theory.

The ambiguous sign  $\pm$  in (2.9) defines different regions in the phase space  $\Gamma$ . In particular, only the choice of a plus sign includes the special case of a homogeneous and isotropic geometry coupled to a scalar field. In the case of the minus sign specialized to cosmological spacetimes, where each vector constraint vanishes identically, the expression for  $\pi^2$  above will just yield zero on the right-hand side.

### B. A deparametrized model

What we have done in the last section is solve the scalar constraint for the scalar field momentum by using the vector constraint. Physically, this corresponds, as will be explained more in detail below, to choose the scalar field  $\phi$  as our emergent time with respect to which the dynamics of the observables will be formulated. This calculation provides the relation between the standard real scalar field coupled to gravity, on the one hand, and the model we actually *define* below, on the other hand.

In our paper we will consider a model that is defined by the vector constraint (2.5), the Gauss constraint (2.7), and the following scalar constraint:

$$C'(x) = \pi(x) - h(x), \quad (2.10)$$

$$h := \sqrt{-\sqrt{q}C^{\text{gr}} + \sqrt{q}\sqrt{(C^{\text{gr}})^2 - q^{ab}C_a^{\text{gr}}C_b^{\text{gr}}}}. \quad (2.11)$$

The scalar constraint  $C(x)$  has been rewritten using (2.9). That theory is equivalent to the theory defined in the previous subsection in the case of no potential

$$V(\phi) = 0 \quad (2.12)$$

and in the region of the phase space  $\Gamma$  such that “+” holds in (2.9) and

$$\pi > 0. \quad (2.13)$$

Since the potential is set to zero in the model,  $\phi$  no longer occurs in the function  $h$  and the scalar constraints deparametrize. Notice that in the consequence of the constraints, in that region

$$C^{\text{gr}} < 0. \quad (2.14)$$

The deparametrized scalar constraints, being linear in the scalar field momentum, strongly Poisson commute

$$\{C'(x), C'(y)\} = 0, \quad (2.15)$$

as a consequence of the following identity:

$$\{h(x), h(y)\} = 0 \quad (2.16)$$

proved in [24]. A Dirac observable is the restriction to the constraint surface of a function  $f: \Gamma \rightarrow \mathbb{R}$ , such that

$$\{f, C_a(x)\} = \{f, C'(x)\} = \{f, G_a^i(x)\} = 0. \quad (2.17)$$

The vanishing of the first Poisson bracket means that  $f$  is invariant with respect to the action of the local diffeomorphisms (that is, all diffeomorphisms generated by the

vector fields tangent to  $M$ ), and the vanishing of the third Poisson bracket is equivalent to the Yang-Mills gauge invariance of  $f$ . The vanishing of the second Poisson bracket reads

$$\{f, \pi(x)\} = \{f, h(x)\}. \quad (2.18)$$

### III. QUANTUM CANONICAL GRAVITY COUPLED TO A SCALAR FIELD

In this section we introduce a “formal” structure of our theory. Our goal, at this point, is to conclude what mathematical structures (Hilbert spaces, operators, etc.) are needed to complete the quantization of the model. How to construct them using LQG will be explained in the next section.

Assuming for the time being that all Hilbert spaces and operators we need exist, and that they have the usual properties, we will now derive:

- (i) a general solution to the quantum constraints,
- (ii) a general quantum Dirac observable, its classical interpretation, and its physical evolution,
- (iii) the Hilbert product between two solutions.

#### A. Quantum states and quantum fields

The quantum states are complex valued functions

$$(\phi, A) \mapsto \Psi(\phi, A), \quad (3.1)$$

where  $\phi$  and  $A$  are the scalar field and the Ashtekar-Barbero connection defined on  $M$  in the previous section (henceforth, we will write  $A$  and  $P$  instead of  $A_a^i$  and  $P_i^a$ ).

For a given representation the fields  $\phi$ ,  $\pi$ ,  $A$ ,  $P$  give rise to quantum operators

$$\begin{aligned} \hat{\phi}(x)\Psi(\phi, A) &= \phi(x)\Psi(\phi, A), \\ \hat{\pi}(x)\Psi(\phi, A) &= \frac{1}{i} \frac{\delta}{\delta\phi(x)} \Psi(\phi, A), \end{aligned} \quad (3.2)$$

$$\begin{aligned} \hat{A}_b^j(x)\Psi(\phi, A) &= A_b^j(x)\Psi(\phi, A), \\ \hat{P}_j^b(x)\Psi(\phi, A) &= \frac{1}{i} \frac{\delta}{\delta A_b^j(x)} \Psi(\phi, A). \end{aligned} \quad (3.3)$$

These elementary operators are needed to define the operators corresponding to the classical constraints and to define the quantum observables.

#### B. The quantum constraints and their solutions

We turn now to the quantum constraints and their solutions. The first step is defining the quantum counterparts of the classical constraints (2.5), (2.6), and (2.7). In LQG we assume that the quantum Gauss constraints corresponding to the classical expression in (2.7) still generate the “Yang-Mills” gauge transformations; hence their solutions are functions such that

$$\Psi(\phi, a^{-1}Aa + a^{-1}da) = \Psi(\phi, A) \quad (3.4)$$

for every  $a: M \rightarrow \text{SU}(2)$ .

Similarly, we assume that the quantum vector constraints generate the local diffeomorphism transformations of the quantum states, and in the consequence, the quantum vector constraint carries over to the condition that  $\Psi$  be invariant with respect to all local diffeomorphisms  $\varphi: M \rightarrow M$ , that is,

$$\Psi(\varphi^*\phi, \varphi^*A) = \Psi(\phi, A). \quad (3.5)$$

The quantum deparametrized scalar constraint operator has the following form:

$$\hat{C}'(x)\Psi = (\hat{\pi}(x) - \hat{h}(x))\Psi. \quad (3.6)$$

We use Eq. (2.11) (which gives the expression for  $h$  as a functional of  $A$  and  $P$ ) to quantize the second term in the parentheses. Heuristically we get

$$\hat{h}(x) = h(\hat{A}, \hat{P})(x).$$

Because of operator ordering aspects the definition of  $\hat{h}$  is not unique and will be completed later in this paper. In order to avoid a quantum anomaly we must respect the classical symmetry in (2.16) also at the quantum level and must make sure that

$$[\hat{h}(x), \hat{h}(y)] = 0 \quad (3.7)$$

[compare to (2.16)]. Given the quantum constraint operator (3.6), the constraint itself reads

$$(\hat{\pi}(x) - \hat{h}(x))\Psi = 0. \quad (3.8)$$

To solve the quantum deparametrized scalar constraint, we write  $\Psi$  as

$$\Psi = e^{i \int d^3x \hat{\phi}(x) \hat{h}(x)} \psi, \quad (3.9)$$

with a new function  $\psi$ , and insert it in (3.8) to obtain

$$\frac{\delta}{\delta \phi(x)} \Psi(\phi, A) = i \hat{h}(x) \Psi(\phi, A). \quad (3.10)$$

Because of the commutator in (3.7), the constraint equation (3.10) turns into

$$\frac{\delta}{\delta \phi(x)} \psi = 0. \quad (3.11)$$

Hence, a general solution to (3.10) is

$$\Psi(\phi, A) = e^{i \int d^3x \hat{\phi}(x) \hat{h}(x)} \psi(A). \quad (3.12)$$

Notice that the exponentiated operator acting at  $\psi$  on the right-hand side of (3.9) is Yang-Mills gauge and diffeomorphism invariant itself. Therefore, note the following.

A general solution to the quantum vector, Gauss, and scalar constraints is every function (3.12), such that for every local diffeomorphism  $\varphi: M \rightarrow M$ ,

$$\psi(\varphi^*A) = \psi(A), \quad (3.13)$$

and for every  $a: M \rightarrow \text{SU}(2)$

$$\psi(a^{-1}Aa + a^{-1}da) = \psi(A). \quad (3.14)$$

In the remaining part of the article we will be using the abbreviation

$$\int d^3x \hat{\phi} \hat{h} := \int d^3x \hat{\phi}(x) \hat{h}(x). \quad (3.15)$$

### C. Quantum Dirac observables

A quantum Dirac observable is the restriction to the space of solutions to the quantum constraints of an operator  $\hat{\mathcal{O}}$  which satisfies the following two properties:

- (i)  $\hat{\mathcal{O}}$  is invariant under local diffeomorphism and Yang-Mills gauge transformations,
- (ii)

$$[\hat{\mathcal{O}}, \hat{C}'(x)] = 0. \quad (3.16)$$

Following the ideas of the relational framework for observables [5–7], it is easy to construct a large family of Dirac observables. Let  $\hat{L}$  be a linear operator which maps the functions  $A \mapsto \psi(A)$  into functions  $A \mapsto \hat{L}\psi(A)$ . Consider an operator

$$\mathcal{O}(\hat{L}) := e^{i \int d^3x \hat{\phi} \hat{h}} \hat{L} e^{-i \int d^3x \hat{\phi} \hat{h}}. \quad (3.17)$$

As required, the operator  $\mathcal{O}(\hat{L})$  commutes with the quantum version of the deparametrized scalar constraints,

$$[\mathcal{O}(\hat{L}), \hat{C}'(x)] = 0. \quad (3.18)$$

Moreover, the operator  $\mathcal{O}(\hat{L})$  is Yang-Mills gauge and local diffeomorphism invariant provided the operator  $\hat{L}$  is.

Each of the operators  $\mathcal{O}(\hat{L})$  defined by a Yang-Mills gauge and diffeomorphism invariant operator  $\hat{L}$  preserves the space of solutions to the constraints. Indeed,

$$\mathcal{O}(\hat{L}) e^{i \int d^3x \hat{\phi} \hat{h}} \psi(A) = e^{i \int d^3x \hat{\phi} \hat{h}} \psi'(A), \quad \psi' = \hat{L}\psi. \quad (3.19)$$

The operators (3.19) with the Yang-Mills gauge and local diffeomorphism invariant operators  $\hat{L}$  set a family (algebra, modulo the domains) of the Dirac observables. The total scalar field momentum  $\int_M d^3x \hat{\pi}(x)$  also defines one of the quantum Dirac observables (3.19), namely

$$\mathcal{O}\left(\int_M d^3x \hat{h}(x)\right) = \int_M d^3x \hat{h}(x). \quad (3.20)$$

The family of the Dirac observables (3.19), in fact, contains *all* the quantum Dirac observables. To see that

this is true, suppose an operator  $\hat{\mathcal{O}}$  satisfies the condition (3.16) at each  $x \in M$ . Let us write the operator in the following way:

$$\hat{\mathcal{O}} = e^{i \int d^3x \hat{\phi} \hat{h}} \hat{K} e^{-i \int d^3x \hat{\phi} \hat{h}}, \quad (3.21)$$

where  $\hat{K}$  is the *a priori* arbitrary operator. The condition (3.16) with  $\hat{\mathcal{O}}$  substituted for the right-hand side of (3.21) takes the following form:

$$[\hat{K}, \hat{\pi}(x)] = 0. \quad (3.22)$$

The set of all the solutions  $\hat{K}$  to (3.22) is generated by the following solutions: (i) given any  $x \in M$ ,

$$\hat{K} = \hat{\pi}(x),$$

and (ii)

$$\hat{K} = \hat{L},$$

considered above, that is,  $\hat{L}$ , which maps the functions  $A \mapsto \psi(A)$  into functions  $A \mapsto \hat{L}\psi(A)$ .

The solutions of type (ii) give rise exactly to the family of the quantum Dirac observables (3.19) we have introduced above. On the other hand, a solution of type (i) gives rise to the following quantum Dirac observable:

$$e^{i \int d^3x \hat{\phi} \hat{h}} \hat{\pi}(x) e^{-i \int d^3x \hat{\phi} \hat{h}} = \hat{\pi}(x) - \hat{h}(x). \quad (3.23)$$

However, we should keep in mind that what really defines a quantum Dirac observable is the restriction to the space of solutions to the quantum constraints. The restriction of (3.23) is identically zero. This shows that all the quantum Dirac observables are those defined by (3.19) and diffeomorphism and Young-Mills invariant operator  $\hat{L}$ .

#### D. Classical interpretation of the Dirac observables

Suppose that a given operator  $\hat{L}$  used to construct the Dirac observable  $\mathcal{O}(\hat{L})$  corresponds in the quantum theory to a classical function  $L$  defined on the gravitational phase space  $\Gamma_{\text{gr}}$ , and that the support of  $L$  is contained in the set on which

$$C^{\text{gr}} < 0. \quad (3.24)$$

To find a classical observable  $\mathcal{O}(L)$  whose quantum counterpart is  $\mathcal{O}(\hat{L})$ , it is convenient to express the operator (3.26) in terms of a formal power series given by

$$\mathcal{O}(\hat{L}) = \sum_{n=0}^{\infty} \frac{i^n}{n!} \left[ \hat{L}, \int d^3x \hat{\phi} \hat{h} \right]_{(n)}, \quad (3.25)$$

where  $[\cdot, \cdot]_{(n)}$  denotes the iterated commutator defined by  $[\hat{L}, \int d^3x \hat{\phi} \hat{h}]_{(0)} = \hat{L}$  and  $[\hat{L}, \int d^3x \hat{\phi} \hat{h}]_{(n)} = [[\hat{L}, \int d^3x \hat{\phi} \hat{h}]_{(n-1)}, \int d^3x \hat{\phi} \hat{h}]$ . The usual substitution  $[\cdot, \cdot] \mapsto -i\{\cdot, \cdot\}$  leads to a formal series

$$\mathcal{O}(L) = \sum_{n=0}^{\infty} \frac{1}{n!} \left\{ L, \int d^3x \phi h \right\}_{(n)} \quad (3.26)$$

for a classical observable  $\mathcal{O}(L)$ . That series is very well known in the theory of relational observables [6–8,22]. To recall its meaning we first consider a slightly more general expression with  $\phi$  replaced by a point dependent parameter  $M \ni x \mapsto t(x)$ , namely,

$$\alpha_t^*(L) = \sum_{n=0}^{\infty} \frac{1}{n!} \left\{ L, \int d^3x t h \right\}_{(n)}. \quad (3.27)$$

The  $*$  denotes the pullback, and the map

$$\alpha_t: \Gamma_{\text{gr}} \rightarrow \Gamma_{\text{gr}}$$

is defined by the Hamiltonian flow  $\beta_t: \Gamma \rightarrow \Gamma$  generated in the full phase space  $\Gamma$  by the constraints  $C'(x)$  with the parameters  $t(x)$ . The action of the flow reads

$$\beta_t(A, P, \phi, \pi) = (\alpha_t(A, P), \phi - t, \pi).$$

Clearly

$$\beta_\phi(A, P, \phi, \pi) = (\alpha_\phi(A, P), 0, \pi). \quad (3.28)$$

The value of  $\mathcal{O}(L)$  at any point  $(A, P, \phi, \pi)$  is defined to be

$$\mathcal{O}(L)(A, P, \phi, \pi) = L(\alpha_\phi(A, P)). \quad (3.29)$$

In conclusion, the quantum Dirac observable  $\mathcal{O}(\hat{L})$  corresponds to the classical function that is also an observable,  $\mathcal{O}(L)$ ,

$$\widehat{\mathcal{O}(L)} = \mathcal{O}(\hat{L}). \quad (3.30)$$

At this point a comment about the status of the operator  $\mathcal{O}(\hat{L})$  is appropriate. It may happen that given a point  $(A, P, \phi, \pi)$  in the classical phase space, the series (3.26) is nonconverging. In fact, we encounter cases like that in the LQC models of a homogeneous isotropic universe with a positive cosmological constant [30]. However, still the operator  $\mathcal{O}(\hat{L})$  is well defined as long as a self-adjoint extension for the operator  $\int d^3x \hat{\phi} \hat{h}$  is fixed, and therefore the unitary operator  $\exp(i \int d^3x \hat{\phi} \hat{h})$  is well defined. Then, the quantum evolution just goes beyond the classical theory. That is exactly the reason we have chosen to define the Dirac observables directly in the quantum theory, and only interpret them in the classical theory as secondary objects.

#### E. Dynamical evolution of the observables

The Dirac observables we have defined are relational observables (often called partial [5,6], Sec. I.2 of [2]). For that class of observables one is able to define a nonvanishing evolution generated by a so-called physical Hamiltonian, which will be introduced in the next section. The dynamics is defined with respect to an internal time given by the values, which that field  $\phi$  takes while being transformed along its gauge orbit. This can be seen in the

construction of the quantity  $\mathcal{O}(L)$  from a given function  $L$  by generalizing the choice of the evaluation point from (3.28) to

$$\beta_{\phi-\phi_0}(A, P, \phi, \pi) = (\alpha_{\phi-\phi_0}(A, P), \phi_0, \pi), \quad (3.31)$$

where  $\phi_0$  is an arbitrarily fixed function on  $M$ . We denote the resulting function defined on the phase space  $\Gamma$  by  $\mathcal{O}_{\phi_0}(L)$ , that is,

$$\mathcal{O}_{\phi_0}(L)(A, P, \phi, \pi) = L(\alpha_{\phi-\phi_0}(A, P)). \quad (3.32)$$

For the function  $\mathcal{O}_{\phi_0}(L)$  to be well defined, the flow  $\beta_t: \Gamma \rightarrow \Gamma$  has to be well defined for

$$t = \phi - \phi_0$$

in the domain of the function  $L$ .

That classical construction leads to a corresponding quantum operator definition

$$\begin{aligned} \mathcal{O}_{\phi_0}(\hat{L})\Psi(\phi, A) \\ = e^{i \int d^3x (\phi(x) - \phi_0(x)) \hat{h}(x)} \hat{L} e^{-i \int d^3x (\phi(x) - \phi_0(x)) \hat{h}(x)} \Psi(\phi, A), \end{aligned} \quad (3.33)$$

where we used  $\hat{\phi}\Psi(\phi, A) = \phi\Psi(\phi, A)$ . This definition will not enlarge the class of the Dirac observables (3.19); indeed,

$$\mathcal{O}_{\phi_0}(\hat{L}) = \mathcal{O}(\hat{L}') \quad (3.34)$$

with

$$\hat{L}' = e^{-i \int d^3x \phi_0(x) \hat{h}(x)} \hat{L} e^{i \int d^3x \phi_0(x) \hat{h}(x)}. \quad (3.35)$$

In this way, in the algebra of the (formal) solutions to the condition

$$[\hat{O}, \hat{C}'(x)] = 0 \quad (3.36)$$

we have defined an Abelian group of automorphisms labeled by the functions  $\phi_0$  defined on  $M$ , namely,

$$\mathcal{O}(\hat{L}) \mapsto \mathcal{O}_{\phi_0}(\hat{L}). \quad (3.37)$$

If we want to restrict the automorphisms to the algebra of the quantum Dirac observables, we encounter an obstacle. Given a function  $\phi_0$ , we want the operator (3.35) to be diffeomorphism invariant for every diffeomorphism invariant operator  $\hat{L}$ . For the operators  $\hat{h}(x)$  that will be constructed from the LQG framework, that condition can be satisfied only for a constant function,

$$\phi_0(x) = \phi_0 \in \mathbb{R}, \quad \text{for every } x \in M. \quad (3.38)$$

The result is a one-dimensional group of automorphisms of the algebra of the quantum Dirac observables. The group encodes the dependence on the internal time of the algebra of the quantum Dirac observables.

## F. The physical Hamiltonian

The dynamics is generated by the following equation:

$$\frac{d}{d\phi_0} \mathcal{O}_{\phi_0}(\hat{L}) = -i[\hat{h}_{\text{phys}}, \mathcal{O}_{\phi_0}(\hat{L})], \quad (3.39)$$

where

$$\hat{h}_{\text{phys}} := \int d^3x \hat{h}(x) \quad (3.40)$$

is usually called the physical Hamiltonian for the reason that it is a nonvanishing Dirac observable generating true ‘‘physical’’ evolution in contrast to the Hamiltonian constraint.

The physical Hamiltonian will be an exact implementation of the heuristic formula

$$\hat{h}_{\text{phys}} = \int d^3x \sqrt{-\sqrt{\hat{q}} \hat{C}^{\text{gr}} + \sqrt{\hat{q}} \sqrt{(\hat{C}^{\text{gr}})^2 - \hat{q}^{ab} \hat{C}_a^{\text{gr}} \hat{C}_b^{\text{gr}}}}. \quad (3.41)$$

We remember however, that the operator will be applied to diffeomorphism invariant states (3.5), whereas the operator  $\hat{C}_a^{\text{gr}}$  should generate the diffeomorphisms. Therefore, assuming the suitable choice of the ordering, the physical Hamiltonian acting on the diffeomorphism invariant functions  $\psi$  is

$$\hat{h}_{\text{phys}} \psi(A) = \int d^3x \sqrt{-2\sqrt{\hat{q}} \hat{C}^{\text{gr}}} \psi(A), \quad (3.42)$$

where we also took into account [recall (2.14)]

$$\hat{C}^{\text{gr}} < 0. \quad (3.43)$$

This result coincides with that of [23].

## G. The Hilbert product between the solutions: $\mathcal{H}_{\text{phys}}$

Suppose we have a sesquilinear scalar product for the Yang-Mills gauge and local diffeomorphism invariant functions (or distributions) defined on the space of the Ashtekar-Barbero connections. Denote the product of the functions  $\psi$  and  $\psi'$  by

$$(\psi | \psi'), \quad (3.44)$$

and the corresponding Hilbert space by  $\mathcal{H}_{\text{diff}}$ .

We can use it to define the physical (that is, respecting the dynamics) Hilbert product in the space of solutions (3.12):

$$(e^{i \int \hat{\phi} \hat{h}} \psi | e^{i \int \hat{\phi} \hat{h}} \psi')_{\text{phys}} := (\psi | \psi'). \quad (3.45)$$

The resulting Hilbert space  $\mathcal{H}_{\text{phys}}$  is physical, and its elements are the physical states.

## H. Summary: The exact structures we need

In summary, in order to construct the quantum model we will need:

- (i) the Hilbert space  $\mathcal{H}_{\text{diff}}$  of the Yang-Mills gauge and the local diffeomorphism invariant quantum states of geometry,
- (ii) the operators in  $\mathcal{H}_{\text{diff}}$ , which admit a well-understood geometric interpretation,
- (iii) the physical Hamiltonian operator  $\hat{h}_{\text{phys}}$  defined in a suitable domain in  $\mathcal{H}_{\text{diff}}$  (which is not expected to be dense, because the heuristic formula for the operator involves the square roots of nondefinite expressions).

Given all that, the physical Hilbert space is unitarily isomorphic via

$$e^i \int d^3x \hat{\phi} \hat{h} \psi \mapsto \psi \quad (3.46)$$

with the domain of  $\hat{h}_{\text{phys}}$  in  $\mathcal{H}_{\text{diff}}$ .

Every observable  $\mathcal{O}(\hat{L})$  (for simplicity let  $\hat{L}$  be bounded) is the pullback by (3.46) of an operator  $\hat{L}$ , which preserves the completion of the domain of  $\hat{h}_{\text{phys}}$ .

Finally, the emerged dynamical evolution (3.39) of the observables reads

$$\hat{L}(\tau) = e^{-i\tau\hat{h}_{\text{phys}}} \hat{L} e^{i\tau\hat{h}_{\text{phys}}}. \quad (3.47)$$

This is precisely the very well-known Heisenberg picture evolution defined by the Hamiltonian  $\hat{h}_{\text{phys}}$ .

Notice that, in fact, it is not necessary for  $\hat{L}$  to preserve the domain of  $\hat{h}_{\text{phys}}$ . Indeed, given any  $\psi$  in that domain, the expectation value

$$\langle \psi | e^{-i\tau\hat{h}_{\text{phys}}} \hat{L} e^{i\tau\hat{h}_{\text{phys}}} \psi \rangle = \langle e^{i\tau\hat{h}_{\text{phys}}} \psi | \hat{L} e^{i\tau\hat{h}_{\text{phys}}} \psi \rangle$$

is well defined. This can be seen by using that it is equivalent to replace  $\hat{L}$  by the operator

$$\hat{L}' = P\hat{L}P, \quad (3.48)$$

where  $P$  is the orthogonal projection onto the completion of the domain of  $\hat{h}_{\text{phys}}$ , and to considering the pullback of the Dirac observable  $\mathcal{O}(\hat{L}')$  together with its dynamics.

This kind of structure will be necessary for the outcome. This is all we need to complete the quantization of a model of quantum gravity coupled to a scalar field.

In the derivation of the operator corresponding to the physical Hamiltonian  $\hat{h}_{\text{phys}}$ , however, we will need yet more structure:

- (i) the operator  $\hat{h}_{\text{phys}}$  should be defined by using the suitably defined operator valued distribution  $M \ni x \mapsto \widehat{\sqrt{q}(x)} C^{\text{gr}}(x)$ ,
- (ii) the distribution should be self-adjoint, so that we can use the spectral decomposition to define the subspace

$$\widehat{\sqrt{q}(x)} C^{\text{gr}}(x) < 0 \quad (3.49)$$

and thereon the new operator valued distribution

$$\hat{h}(x) = \sqrt{-2\sqrt{q}(x)C^{\text{gr}}(x)}, \quad (3.50)$$

- (iii) we should be able to verify the condition

$$[\hat{h}(x), \hat{h}(y)] = 0, \quad (3.51)$$

- (iv) and finally define

$$\hat{h}_{\text{phys}} = \int d^3x \hat{h}(x). \quad (3.52)$$

Notice, that none of the operators  $\sqrt{q}(x)C^{\text{gr}}(x)$  or  $\hat{h}(x)$  can be defined within the Hilbert space  $\mathcal{H}_{\text{diff}}$ , because the  $x$  dependence manifestly breaks the diffeomorphism invariance. Therefore, the properties of the self-adjointness require some extra Hilbert spaces,  $\mathcal{H}_{\text{diff},x}$ , labeled by the points of  $M$ , whereas the commuting at different points can be defined only on a yet bigger Hilbert space.

Remarkably, all the suitable structures can be constructed within the LQG framework, as we will explain in the next section.

## IV. APPLICATION OF LQG

### A. The Hilbert spaces

#### 1. The kinematical Hilbert space of quantum states of the geometry

In LQG (we use the notation of [4]), the kinematical Hilbert space of quantum states of the geometry is set by the so-called cylindrical functions of the connection  $A$ . A cylindrical function is defined by a set  $\alpha$  of finite curves  $e_1, \dots, e_n$  in  $M$  and by a continuous function  $f: \text{SU}(2)^n \rightarrow \mathbb{C}$ , in the following way:

$$\psi_{\alpha,f}(A) = f(A(e_1), \dots, A(e_n)), \quad (4.1)$$

where the symbol  $A(e)$  denotes the parallel transport along  $e$  defined by the connection  $A$ . The set  $\text{Cyl}$  of the cylindrical functions is a vector space, and an associative algebra. The space of the cylindrical functions  $\text{Cyl}$  is endowed with an integral

$$\psi_{\alpha,f} \mapsto \int \psi_{\alpha,f} \quad (4.2)$$

used to define the sesquilinear scalar product

$$\langle \psi_{\alpha,f} | \psi_{\alpha',f'} \rangle_{\text{gr}} = \int \bar{\psi}_{\alpha,f} \psi_{\alpha',f'}, \quad (4.3)$$

and defines (after the completion) the kinematical Hilbert space  $\mathcal{H}$  for the geometric operators in LQG. We assume in this paper that the manifold and the curves are piecewise analytic. Then, for every cylindrical function there exist curves  $\alpha = \{e_1, \dots, e_n\}$ , which form a graph embedded in  $M$  (that is, they are allowed to intersect only at the ends)

such that the function is given by (4.1). The curves  $e_I$  are called edges of the given graph  $\alpha$ .<sup>2</sup>

For a cylindrical function defined by a graph, we have

$$\int \psi_{\alpha,f} = \int_{\text{SU}(2)^n} d^n g f(g_1, \dots, g_n), \quad (4.4)$$

where  $d^n g$  is the Haar measure on  $\text{SU}(2)^n$ . The geometric operators preserving the space  $\text{Cyl}$  are

$$\hat{A}(e)_C^B \psi_{\alpha,f}(A) = A(e)_C^B f(A(e_1), \dots, A(e_n)) \quad (4.5)$$

and

$$\int_S \hat{P}_i^a \psi_{\alpha,f} = \frac{1}{2i} \int_S \frac{\delta}{\delta A_i^a} \psi_{\alpha,f} \eta_{abc} dx^b \wedge dx^c. \quad (4.6)$$

There is an orthogonal decomposition of  $\mathcal{H}$  into subspaces  $\mathcal{H}'_\alpha$  labeled by the embedded graphs  $\alpha$ . To define it, denote first by (unprimed)  $\mathcal{H}_\alpha \subset \mathcal{H}$  the Hilbert subspace spanned by the cylindrical functions  $\psi_{\alpha,f}$ , with all the possible functions  $f$ . Those spaces, however, are too big to provide the orthogonal decomposition. Given a graph  $\alpha$ , whenever a graph  $\beta$  can be obtained from the edges of  $\alpha$  by glueing, or reversing the orientation or removing some of them, then  $\mathcal{H}_\beta \subset \mathcal{H}_\alpha$ . Therefore, define  $\mathcal{H}'_\alpha \subset \mathcal{H}_\alpha$  to be the orthogonal complement in  $\mathcal{H}_\alpha$  of the subspace spanned by those subspaces  $\mathcal{H}_\beta$ . The decomposition is

$$\mathcal{H} = \bigoplus_{\alpha} \mathcal{H}'_{\alpha}, \quad (4.7)$$

where  $\alpha$  runs through the set of all the semianalytic embedded graphs in  $M$ .

## 2. The Hilbert space of the diffeomorphism invariant states of the geometry

Semianalytic diffeomorphisms  $\text{Diff}(M)$  of  $M$  preserve the space  $\text{Cyl}$  and act unitarily in the Hilbert space  $\mathcal{H}$  just by the natural pullback of the Ashtekar-Barbero connections. Denote the action of  $\varphi \in \text{Diff}(M)$  by

$$U_\varphi: \mathcal{H} \rightarrow \mathcal{H}. \quad (4.8)$$

To implement the construction of the quantum operator corresponding to the physical Hamiltonian, we will need two different Hilbert spaces: One of them includes states that are invariant with respect to all (semianalytic) local diffeomorphisms  $\text{Diff}(M)$  of  $M$ , and the other one is the home of the states invariant with respect to the subgroup  $\text{Diff}(M, x)$ , which preserves a given point  $x \in M$ . (Later, we will also impose the Gauss constraint, which is the condition of Yang-Mills gauge invariance.) Let ‘‘Diff’’

stand for either  $\text{Diff}(M)$  or  $\text{Diff}(M, x)$ . The only Diff invariant direction in  $\mathcal{H}$  is the constant function. However, since the group Diff is not compact, we expect the invariant states to be distributions on the space of the Ashtekar-Barbero connections, that is, linear maps

$$\langle \Psi | : \text{Cyl} \rightarrow \mathbb{C}. \quad (4.9)$$

Whereas the space of all distributions seems to be too big, a suitable rigging map can be defined, which carries each  $\psi \in \text{Cyl}$  into a Diff invariant distribution  $\eta_{\text{Diff}}(\psi)$ . To recall the definition of this map, we need the orthogonal decomposition (4.7). The map  $\eta_{\text{Diff}}$  is introduced for each subspace  $\mathcal{H}'_\alpha$  individually. By the linearity, it extends to every cylindrical function. That is, the domain of the rigging map  $\eta_{\text{Diff}}$  is  $\text{Cyl} \subset \mathcal{H}$ . The first step in the construction of the rigging map  $\eta_{\text{Diff}}$  is identification of the elements of  $\mathcal{H}'_\alpha$  that will be annihilated. Consider those diffeomorphisms  $\varphi \in \text{Diff}$ , which map each edge of  $\alpha$  into another edge modulo of the orientation, and let us call them the symmetries of  $\alpha$  and denote their group by  $\text{Diff}\alpha$ . The functions  $\psi \in \mathcal{H}'_\alpha$  invariant with respect to  $\text{Diff}\alpha$  form a subspace denoted by either  $\mathcal{H}'_{\alpha, \text{inv}}$  in the  $\text{Diff} = \text{Diff}(M)$  case or  $\mathcal{H}'_{\alpha, \text{inv}, x}$  in the case of  $\text{Diff} = \text{Diff}(M, x)$ . The elements of  $\mathcal{H}'_\alpha$  orthogonal to  $\mathcal{H}'_{\alpha, \text{inv}}$  are annihilated by the rigging map  $\eta_{\text{Diff}}$ . For  $\psi \in \mathcal{H}'_{\alpha, \text{inv}}$ ,  $\eta_{\text{Diff}}(\psi)$  is defined as follows:

$$\eta_{\text{Diff}}(\psi): \psi'' \mapsto \sum_{[\phi] \in \text{Diff}/\text{Diff}\alpha} (U_\phi \psi | \psi''). \quad (4.10)$$

Note that if  $\psi'' \in \mathcal{H}'_{\alpha''}$ , then the right-hand side is zero if  $\alpha''$  is not Diff equivalent to  $\alpha$ , and in the case there is  $\phi'' \in \text{Diff}$  such that

$$\phi''(\alpha) = \alpha'', \quad (4.11)$$

the only possibly nonzero term in the sum in (4.10) is

$$\eta_{\text{Diff}}(\psi): \psi'' \mapsto (U_{\phi''} \psi | \psi''). \quad (4.12)$$

Since every cylindrical function is a finite sum of elements of the Hilbert spaces  $\mathcal{H}'_\alpha$ ,  $\eta_{\text{Diff}}(\psi)$  is defined in  $\text{Cyl}$ . For the same reason, the map

$$\psi \eta_{\text{Diff}}(\psi) \quad (4.13)$$

extends by the finite linearity to  $\text{Cyl}$ .

With the rigging map  $\eta_{\text{Diff}}$  we define not only the vector space of the Diff invariant states to be the image  $\eta_{\text{Diff}}(\text{Cyl})$ , but also the sesquilinear product

$$(\eta_{\text{Diff}}(\psi) | \eta_{\text{Diff}}(\psi'))_{\text{Diff}} := \langle \eta_{\text{Diff}}(\psi), \psi' \rangle. \quad (4.14)$$

In this way we have defined a Hilbert space  $\mathcal{H}_{\text{Diff}}$ . The map  $\eta_{\text{Diff}}$  defines a natural isometry

$$\mathcal{H}_{\text{Diff}} \equiv \bigoplus_{[\alpha]} \mathcal{H}'_{\alpha, \text{Diff}}, \quad (4.15)$$

<sup>2</sup>To be more precise, in what follows, an edge is either an oriented semianalytic embedding of a circle in  $M$  or a parametrization-free, oriented, finite curve defined by  $e: [0, 1] \rightarrow M$  such that either  $e$  is an embedding or  $e(0) = e(1)$ .

where  $[\alpha]$  runs through the set of the Diff classes of the graphs embedded in  $M$ . Recall that  $\text{Diff} = \text{Diff}(M)$ ,  $\text{Diff}(M, x)$ . Therefore, we have defined two types of the Hilbert spaces: the Hilbert  $\mathcal{H}_{\text{Diff}(M)}$  and, respectively, per each point  $x \in M$ , the Hilbert space  $\mathcal{H}_{\text{Diff}(M, x)}$ .

### 3. The Hilbert spaces of the Yang-Mills gauge and diffeomorphism invariant states of the geometry

Imposing the Gauss constraint is yet easier than requiring diffeomorphism invariance, and could be equivalently done either before or after solving the diffeomorphism constraint. The group of unitary transformations of  $\mathcal{H}$  given by the Yang-Mills gauge transformations is compact. Hence all solutions to the Gauss constraint in  $\mathcal{H}$  are invariant elements of  $\mathcal{H}$  (as opposed to non-normalizable states, distributions). Moreover, the group of the Yang-Mills gauge transformations (3.4) preserves each of the subspaces  $\mathcal{H}'_\alpha$ . For every Yang-Mills gauge invariant  $\psi \in \text{Cyl}$ , the Diff invariant distribution

$$\eta_{\text{Diff}}(\psi) \in \mathcal{H}_{\text{Diff}} \quad (4.16)$$

is also insensitive to gauge transformations of  $\psi'' \in \text{Cyl}$ . Namely, the number

$$\eta_{\text{Diff}}(\psi)(\psi'')$$

is invariant. The converse is also true: If  $\eta_{\text{Diff}}(\psi)(\psi'')$  is invariant with respect to the Yang-Mills gauge transformations of  $\psi''$ , then  $\psi$  is Yang-Mills gauge invariant.

In conclusion, the Yang-Mills gauge and diffeomorphism invariant distributions on the space of the Ashtekar-Barbero connections we want to use to construct the Hilbert space  $\mathcal{H}_{\text{diff}}$  of Sec. III G are the distributions

$$\eta_{\text{Diff}(M)}(\psi) \quad (4.17)$$

obtained from the Yang-Mills gauge invariant cylindrical functions  $\psi$ . Denote their Hilbert space by  $\mathcal{H}_{\text{diff}}$ . By construction

$$\mathcal{H}_{\text{diff}} \subset \mathcal{H}_{\text{Diff}(M)}. \quad (4.18)$$

For the introduction of the physical Hamiltonian we will also use the Hilbert space  $\mathcal{H}_{\text{diff}, x}$  obtained by replacing in the construction of the Hilbert space  $\mathcal{H}_{\text{diff}}$  the group  $\text{Diff}(M)$  by the group  $\text{Diff}(M, x)$ .

## B. The operators

### 1. The Dirac observables

From the previous subsection we already have the LQG candidate for the Hilbert space  $\mathcal{H}_{\text{diff}}$  of the Yang-Mills gauge invariant and diffeomorphism invariant quantum states of geometry. As we already know from Sec. III G, from a suitable subspace of this space we will construct the physical Hilbert space of solutions to all the constraints of the model we are considering. Second, in the Hilbert space  $\mathcal{H}_{\text{diff}}$  we will need the operators representing the

geometry of the initial data defined on  $M$ , from which we will construct the Dirac observables.

Let us begin with this second task, because it is easier. We assume below that the operators we consider in the Hilbert space  $\mathcal{H}$  as the domain have the vector subspace  $\text{Cyl}$  of the cylindrical functions. Every Yang-Mills gauge and  $\text{Diff}(M)$  symmetric operator  $\tilde{L}$  defined in the kinematical Hilbert space  $\mathcal{H}$  defines naturally by the duality a symmetric operator  $\hat{L}$  in  $\mathcal{H}_{\text{diff}}$ ,

$$\begin{aligned} \langle \hat{L} \eta_{\text{Diff}(M)}(\psi), \psi'' \rangle &:= \langle \eta_{\text{Diff}(M)}(\psi), \tilde{L} \psi'' \rangle \\ &= \langle \eta_{\text{Diff}(M)}(\tilde{L} \psi), \psi'' \rangle, \end{aligned} \quad (4.19)$$

where the bracket is the action of a distribution (a first entry) into a given cylindrical function  $\psi''$ ; that is, we could phrase it in a simpler way,

$$\hat{L} \eta_{\text{Diff}(M)}(\psi) = \eta_{\text{Diff}(M)}(\hat{L} \psi). \quad (4.20)$$

An excellent example of a Yang-Mills gauge and diffeomorphism invariant operator in  $\mathcal{H}$  available in the literature [4,31] is the volume of the underlying manifold  $M$  operator

$$\tilde{V}_M = \int d^x \tilde{\sqrt{q}}(x). \quad (4.21)$$

Another example we manage to construct might be any quantum operator representing the integral of a scalar constructed from the intrinsic or extrinsic curvature.

In the kinematical Hilbert space  $\mathcal{H}$ , there is also a well-defined operator valued distribution

$$\tilde{\sqrt{q}}(x) = \sum_{x' \in M} \delta(x, x') \tilde{\sqrt{q}}_{x'}, \quad (4.22)$$

where each of the operators  $\tilde{\sqrt{q}}_{x'}$  is  $\text{Diff}(M, x')$  invariant. The uncountable sum on the right-hand side is well defined, because for every smearing function  $F: M \rightarrow \mathbb{R}$ , and a cylindrical function  $\psi_{\alpha, f}$ , we have

$$\int d^3x F(x) \tilde{\sqrt{q}}(x) \psi_{\alpha, f} = \sum_{I=1}^n F(v_I) \tilde{\sqrt{q}}_{v_I} \psi_{\alpha, f}, \quad (4.23)$$

where  $v_1, \dots, v_n$  are the vertices of the graph  $\alpha$ . Via (4.20), for every  $x' \in M$ , the operator  $\tilde{\sqrt{q}}_{x'}$  defines an operator  $\hat{\sqrt{q}}_{x'}$  in  $\mathcal{H}_{\text{diff}, x'}$ . Morally,  $\tilde{\sqrt{q}}(x)$  is also  $\text{Diff}(M, x)$  invariant for every given  $x \in M$ ; therefore (4.20) should also be somehow generalized to this case. Indeed (see [32]), the suitable generalization is natural and provides in this case a distribution

$$\hat{\sqrt{q}}(x) = \sum_{x' \in M} \delta(x, x') \hat{\sqrt{q}}_{x'}, \quad (4.24)$$

which makes sense due to the fact that all the Hilbert spaces  $\mathcal{H}_{\text{diff}, x}$  are embedded in the single vector space  $\text{Cyl}^*$ .

There is one more technical remark in order at this point. Consider two operator valued distributions in  $\mathcal{H}$ , of the form

$$\tilde{A}(x) = \sum_{x' \in M} \delta(x, x') \tilde{A}_{x'}, \quad \tilde{B}(x) = \sum_{x' \in M} \delta(x, x') \tilde{B}_{x'}, \quad (4.25)$$

each of which satisfies the property (4.23). A natural regularization by smearing leads to a new operator valued distribution

$$\sqrt{\tilde{A}(x)\tilde{B}(x)} = \sum_{x' \in M} \delta(x, x') \sqrt{S(\tilde{A}_{x'}\tilde{B}_{x'})}, \quad (4.26)$$

which also has the property (4.23), where  $S$  stands for a symmetric product of the operators, and the domain of the resulting operator is restricted by the positivity of the  $S(\tilde{A}_x\tilde{B}_x)$  requirement. The regularization consists in the smearing

$$\begin{aligned} \tilde{A}_\epsilon(x) &= \int d^3\tilde{A}(y) \delta_\epsilon(y, x), \\ \tilde{B}_\epsilon(x) &= \int d^3\tilde{B}(y) \delta_\epsilon(y, x), \end{aligned} \quad (4.27)$$

with a smearing function whose support goes uniformly to  $x = y$  as  $\epsilon \rightarrow 0$ , and which goes to the Dirac  $\delta(x, y)$ . The key trick is an observation that for every fixed graph  $\alpha$ , for sufficiently small  $\epsilon$ ,

$$\tilde{A}_\epsilon(x)\tilde{B}_\epsilon(x)\psi_{\alpha,f} = \sum_{l=1}^n (\delta_\epsilon(x, v_l))^2 \tilde{A}_{v_l}\tilde{B}_{v_l}\psi_{\alpha,f}, \quad (4.28)$$

for any cylindrical function  $\psi_{\alpha,f}$ , and moreover, the sum on the right-hand side contains at most one nonzero element. Because of the latter property

$$\sqrt{\tilde{A}_\epsilon(x)\tilde{B}_\epsilon(x)} = \sum_{l=1}^n \delta_\epsilon(x, v_l) \sqrt{\tilde{A}_{v_l}\tilde{B}_{v_l}} \psi_{\alpha,f}, \quad (4.29)$$

provided the square root is well defined itself. Finally,

$$\int d^3xF(x)\sqrt{\tilde{A}_\epsilon(x)\tilde{B}_\epsilon(x)}\psi_{\alpha,f} \rightarrow \sum_{l=1}^n F(v_l)\sqrt{\tilde{A}_{v_l}\tilde{B}_{v_l}}\psi_{\alpha,f}. \quad (4.30)$$

## 2. The quantum scalar constraint and the physical Hamiltonian

As we remember, our first task we can finally turn to now is a construction of the physical Hamiltonian operator

$$\hat{h}_{\text{phys}} = \int d^3x \sqrt{-2\widehat{\sqrt{q}(x)}C^{\text{gr}}(x)} \quad (4.31)$$

defined in  $\mathcal{H}_{\text{diff}}$ .

A quantum scalar constraint  $\hat{C}_{\text{gr}}$  was defined in [33], and its properties and possible generalizations were studied in [4,32]. We will be using here the formulation of the scalar constraint of [4]. In order to use it for our current

construction, we will need a new element. Thus far, the scalar constraint was used as smeared against arbitrary laps function  $\int d^3xN(x)\hat{C}(x)$ , or as the master constraint  $\int d^3x\widehat{\sqrt{q}(x)}^{-1}\hat{C}(x)\hat{C}^\dagger(x)$ , or as a physical Hamiltonian defined after deparametrization with respect to 4 scalar fields. The smeared scalar constraint maps a domain in  $\mathcal{H}_{\text{diff}}$  into  $\text{Cyl}^*$ , and there is no sense in which it could be symmetric or self-adjoint. The master constraint, on the other hand, as well as the physical Hamiltonian after the 4-fold deparametrization, respectively, is defined in the kinematical Hilbert space  $\mathcal{H}$  as a graph-preserving operator. The current case is a new one, and we will need an operator  $\sqrt{-2\widehat{\sqrt{q}(x)}C^{\text{gr}}(x)}$  defined in  $\mathcal{H}_{\text{diff}}$ .

The quantum scalar constraint presented in [4] takes the following form:

$$\int d^3xN(x)\hat{C}(x) = \sum_{x \in M} \hat{C}_x, \quad (4.32)$$

where each of the operators  $\hat{C}_x$  maps its domain contained in  $\mathcal{H}_{\text{diff}}$  into  $\mathcal{H}_{\text{diff},x}$ . However, as it follows from [32], it naturally defines an operator in the corresponding Hilbert space  $\mathcal{H}_{\text{diff},x}$ . The advantage is that only now can we require the symmetry (self-adjointness) of those operators. As defined in [4], the operators  $\hat{C}_x$  come out nonsymmetric. The minor improvement, but necessary for our current work, consists in replacing them by symmetric operators

$$\hat{C}_x^{\text{gr}} = \frac{1}{2}(\hat{C}_x + \hat{C}_x^\dagger) \quad (4.33)$$

and choosing an essentially self-adjoint extension that may be nonunique. Then, the quantum scalar constraint operator we will use for the physical Hamiltonian takes the following form:

$$\hat{C}^{\text{gr}}(x) = \sum_{x' \in M} \delta(x, x') \hat{C}_{x'}^{\text{gr}}. \quad (4.34)$$

On the other hand, we have already considered above the volume density quantum operator written in the similar form,

$$\widehat{\sqrt{q}(x)} = \sum_{x' \in M} \delta(x, x') \widehat{\sqrt{q}_{x'}}. \quad (4.35)$$

At this point, we are in the position to define the operator

$$\sqrt{-2\widehat{\sqrt{q}(x)}C^{\text{gr}}(x)}. \quad (4.36)$$

A regularization in  $\mathcal{H}$  similar to the one discussed above gives (modulo the symmetrization of the product of the operators  $\widehat{\sqrt{q}_{x'}}$  and  $\hat{C}_{x'}^{\text{gr}}$ )

$$\begin{aligned} \sqrt{-2\widehat{q}(x)C^{\text{gr}}(x)} &= \sum_{x' \in M} \delta(x, x') \sqrt{-2\widehat{q}_{x'}^{1/2} \widehat{C}_{x'}^{\text{gr}} \widehat{q}_{x'}^{1/2}} \\ &=: \widehat{h}(x). \end{aligned} \quad (4.37)$$

However, the operator is well defined only in the subspace of  $\mathcal{H}_{\text{diff},x}$  corresponding to the positive part of the spectrum of  $\widehat{q}_x^{1/2} \widehat{C}_x^{\text{gr}} \widehat{q}_x^{1/2}$ . To formulate that condition we need to choose a self-adjoint extension of the operator in the case it is not unique. Denote the resulting subspace of  $\mathcal{H}_{\text{diff},x}$  by  $\mathcal{H}_{\text{diff},x+}$ . There is a natural averaging map

$$\eta_M: \mathcal{H}_{\text{diff},x} \rightarrow \mathcal{H}_{\text{diff}}, \quad (4.38)$$

$$\eta_{\text{Diff}(M,x)}(\psi) \mapsto \eta_{\text{Diff}(M)}(\psi). \quad (4.39)$$

The domain of the physical Hamiltonian is

$$\mathcal{H}_{\text{phys}} = \eta_M(\mathcal{H}_{\text{diff},x+}), \quad (4.40)$$

and the formula for the physical Hamiltonian reads

$$\widehat{h}_{\text{phys}} = \int d^3x \widehat{h}(x) = \sum_{x \in M} \sqrt{-2\widehat{q}_x^{-1/2} \widehat{C}_x^{\text{gr}} \widehat{q}_x^{-1/2}}. \quad (4.41)$$

We remember the anomaly-free condition (3.51) that should be satisfied by our construction. In [32] an extension of the Hilbert space  $\mathcal{H}_{\text{phys}}$  is introduced in which the smeared scalar constraint operators

$$\widehat{C}^{\text{gr}}(N) = \int_M d^3x N(x) \widehat{C}^{\text{gr}}(x) \quad (4.42)$$

are defined and their products

$$\widehat{C}^{\text{gr}}(N) \widehat{C}^{\text{gr}}(N') \quad (4.43)$$

are contained. It follows from the results of [32] that the smeared constraint operators commute

$$[\widehat{C}^{\text{gr}}(N), \widehat{C}^{\text{gr}}(N')] = 0 \quad (4.44)$$

on a large subspace of the enlarged vector space. It justifies our conjecture that the condition

$$[\widehat{h}(x), \widehat{h}(y)] = 0 \quad (4.45)$$

is a restriction on the ambiguities in the definition of the operators  $\widehat{h}(x)$ , that is, on the loop assignment [2,4] and the self-adjoint extensions.

## V. CONCLUDING REMARKS, OUTLOOK

We have another quantum model of gravity involving all the degrees of freedom. The model discussed here assumes a vanishing potential for the scalar field that becomes the internal time for the Dirac observables. Neglecting this requirement has the effect that the physical Hamiltonian depends on the internal time  $\phi$  as can be seen in Eq. (2.9). Nonconservative Hamiltonians usually

increase the intricacy as far as the technical perspective is concerned. Likewise, if we use, for instance, standard model matter instead of a scalar field, the system will also not deparametrize anymore. Hence, all the technical simplifications due to deparametrization used in this work are not available any longer. A discussion about which kind of matter Lagrangians induce a deparametrization for general relativity can be found in [12].

The quantization of this model is complete and every necessary element exists within the framework of LQG. However, there are still ambiguities present in the LQG definition of the quantum scalar constraint operator due to its nonpolynomial structure. The only way to understand them and their possible physical meaning is to start applying the model. Before explaining what the model discussed in this work is good for, let us compare it briefly to the first model that was completed by Giesel and Thiemann.

### A. Comparison with the Brown-Kuchar model applied to LQG

The Brown-Kuchar (BK) model [9] considers four scalar fields that have the properties of dust and become a dynamically coupled observer, with respect to which the dynamics of the remaining degrees of freedom is formulated. This model was used by Giesel and Thiemann [22], and a reduced phase space of gravity coupled to dust was derived. For this purpose the BK model needed to be extended since the reduced phase space requires also the construction of (classical) Dirac observables with respect to the scalar constraint. The original BK model is rather the counterpart of what is done in this paper because there the vector constraint was reduced classically, whereas for the scalar constraint a quantum condition was formulated.

In the reduced phase space quantization procedure discussed in [22], both, the scalar as well as the diffeomorphism constraint, are reduced classically. The Gauss constraint is, as in this paper, solved at the quantum level. This yields to an algebra of observables describing the classical physical phase space. Because of the deparametrization of the scalar constraints, this algebra turns out to be isomorphic to the kinematical one. In contrast to what is done in this paper, a quantization of the observable algebra accesses directly the physical Hilbert space (once also the Gauss constraint is satisfied). Since the kinematical algebra is isomorphic to the physical one, in [22] the standard kinematical representation of LQG can also be used for the physical Hilbert space  $\mathcal{H}_{\text{phys}}$ . Similar to the work in this paper, the generator of the physical dynamics, the so-called physical Hamiltonian  $h_{\text{phys}}$ , is invariant under local diffeomorphisms. In the reduced approach this leads to the requirement that in order to avoid a quantum anomaly, the operator needs to be invariant under local diffeomorphisms too. As shown in [34] operators being invariant under local diffeomorphisms and defined in the standard (kinematical) LQG representation cannot be graph changing. This means

that they need to preserve the graph they are acting on, yielding the condition that the LQG constraint operators [4,33] entering the physical Hamiltonian  $\hat{h}_{\text{phys}}$  in [22] need to be quantized in a graph-preserving way. As we explained above, LQG is glued from the Hilbert spaces corresponding to all possible graphs. The original LQG scalar constraint operator does not preserve those graph Hilbert spaces. In the model of [22] the physical Hamiltonian must preserve each graph Hilbert space. In the consequence, the constraint operator has to be suitably redefined in [22] when the standard (kinematical) LQG representation is used for  $\mathcal{H}_{\text{phys}}$ . The paper [22] also discusses the quantization of the reduced model in the framework of algebraic quantum gravity [35], where a different representation is used, namely, von Neumann's infinite tensor product representation. The quantum dynamics is not defined on embedded graphs but on abstract ones, carrying only combinatorial information. In this framework only the infinite combinatorial graph that the theory is defined on and that acts like an abstract lattice needs to be preserved by  $\hat{h}_{\text{phys}}$ , whereas any possible subgraph of this does not. In the case of the model presented in this paper here, the graph Hilbert spaces are not preserved and they evolve in the emergent time.

### B. Application of this model

Our model can be used to verify the properties of quantum space-time we expect after learning the lessons from LQC and QFT in curved spacetime.

In the LQC models of the homogeneous massless scalar field coupled to gravity, big bang turns out to be replaced by big bounce, as the result of the quantum gravity effects.

Now, with our model, we can consider the same system of fields from the point of view of the full theory, without the symmetry reduction. Similarly, we can also consider the quantum gravitational collapse, quantum black holes, and theory entropy. All those cases are manageable within our model, and the only difficulty is of a technical nature. Also the Hawking radiation and black hole evaporation process expected from the theory of quantum fields on the classical black hole background are in the range of our model. The next step to obtain progress in this direction is the construction of semiclassical states for full LQG, which are preserved under quantum dynamics generated by the physical Hamiltonian on appropriate time scales.

In conclusion, our paper opens the door to understanding the properties of quantum spacetime from the point of view of the full quantum gravity.

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