

Algebraic quantum gravity (AQG): IV. Reduced phase space quantization of loop quantum gravity

K Giesel^{1,2} and T Thiemann^{3,4}

¹ Excellence Cluster Universe, Technische Universität München, Boltzmannstr. 2, 85748 Garching, Germany

² Nordita, Nordic Institute for Theoretical Physics, Roslagstullsbacken 23, 10691, Stockholm, Sweden

³ University of Erlangen-Nürnberg, Institute for Theoretical Physics III, Staudtstr. 7, 91058, Erlangen, Germany

⁴ Perimeter Institute for Theoretical Physics, 31 Caroline Street N, Waterloo, ON N2 L 2Y5, Canada

E-mail: kristina.giesel@universe-cluster.de, giesel@nordita.org, thiemann@aei.mpg.de and tthiemann@perimeterinstitute.ca

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Abstract

We perform a canonical, reduced phase space quantization of general relativity by loop quantum gravity (LQG) methods. The explicit construction of the reduced phase space is made possible by the combination of (a) the Brown–Kuchař mechanism in the presence of pressure-free dust fields which allows to deparametrize the theory and (b) Rovelli’s relational formalism in the extended version developed by Dittrich to construct the algebra of gauge-invariant observables. Since the resulting algebra of observables is very simple, one can quantize it using the methods of LQG. Basically, the kinematical Hilbert space of non-reduced LQG now becomes a physical Hilbert space and the kinematical results of LQG such as discreteness of spectra of geometrical operators now have physical meaning. The constraints have disappeared; however, the dynamics of the observables is driven by a physical Hamiltonian which is related to the Hamiltonian of the standard model (without dust) and which we quantize in this paper.

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1. Introduction

The objects of ultimate interest in a field theory with gauge symmetry are the gauge-invariant observables. There are two major approaches to the canonical quantization of such theories. In the so-called Dirac approach, one first constructs Hilbert space representations of gauge-variant non-observables and then imposes the vanishing of the quantized version of the classical gauge symmetry generators (constraints) as a selection principle for physical states. The associated

physical Hilbert space then hopefully (if there are no anomalies) carries a representation of the observable algebra. In the so-called reduced phase space approach one first constructs the classical observables and then directly looks for representations of that algebra.

The advantage of the Dirac approach is that the unreduced phase space of non-observables is typically a smooth (Banach) manifold so that the algebra of non-observables is sufficiently simple and representations thereof are easy to construct. Its disadvantage is that one has to deal with spurious degrees of freedom which is the possible source of ambiguities and anomalies in the gauge symmetry algebra. The advantage of the reduced phase space approach is that one never has to care about kinematical Hilbert space representations. However, its disadvantage is that the reduced phase space typically no longer is a smooth manifold turning the induced algebra of observables so difficult that representations thereof are hard to find.

The reduced phase space of general relativity with standard matter is hard to construct explicitly. However, one can combine two independent recent developments in order to make progress.

On the one hand, Brown and Kuchař have shown in a seminal paper [1] that there is hope to construct observables if one adds pressure-free dust to the theory. This is because one can then write the constraints in a deparametrized form⁵.

On the other hand, there is Rovelli's relational formalism [2] for constructing observables which we need in the extended form developed by Dittrich [3]. With this formalism one can write the observables as an infinite series $F_{f;T}$ in terms of powers of the so-called clock variables T and with coefficients involving multiple Poisson brackets between constraints C and non-observables f such that the series is (formally) gauge invariant⁶. Remarkably [3, 4], the map $F_T : f \mapsto F_{f;T}$ is a Poisson homomorphism between the algebra of non-observables f and the algebra of observables with respect to a certain Dirac bracket (which is uniquely determined by the constraints and the functions T).

Now usually Dirac brackets make the Poisson structure so complicated that one cannot find representations thereof. However, as observed in [4], if the system deparametrizes, if one uses as clocks T the configuration variables conjugate to the momenta P in $C = P + H$ and if one considers functions f which do not depend on T , P ⁷ then F_T becomes a Poisson isomorphism. Moreover, the functions H in $C = P + H$ become *physical, conserved Hamiltonian densities* which drive the physical evolution of the observables. This implies that a reduced phase space quantization strategy becomes available, since to find representations of the $F_{f;T}$ is as easy as for the f . The only non-trivial problem left is to find representations which support the physical Hamiltonian⁸.

In [5] these two independent observations were combined and the algebra of classical physical observables was constructed explicitly by adding a general scalar field Lagrangian without potential to the Einstein–Hilbert and standard model Lagrangian. It turns out that among the, in principle, infinite number of physical observables, there is a unique, positive Hamiltonian selected.

In [6, 7] that framework was further improved by using as specific scalar field the pressure-free dust of Brown and Kuchař. The corresponding Hamiltonian is positive, reduces to the

⁵ Given a system of constraints C_I on a phase space, deparametrization means that one can find local coordinates in the form of two mutually commuting sets of canonical pairs (q^a, p_a) , (T^I, π_I) such that the constraints can be written in the locally equivalent form $C_I = \pi_I + H_I$ where the H_I only depend on the (q^a, p_a) .

⁶ It is manifestly gauge invariant in an open neighbourhood of the phase space if the series converges with non-zero convergence radius which has to be checked.

⁷ This is no loss of generality because P can be eliminated in terms of the other degrees of freedom via the constraints and T is pure gauge.

⁸ The caveat is that the deparametrization and thus the reduced phase space quantization is generically only locally valid in phase space. Thus, the globally valid Dirac quantization programme should be developed further in parallel.

ADM energy far away from the sources and to the standard model Hamiltonian on flat space. It generates equations of motion for the observables associated with the non-dust variables that are in agreement with the Einstein equations for the system without dust, up to small corrections which originate from the presence of the dust. In particular one can develop a manifestly gauge-invariant cosmological perturbation theory *to all orders* which was shown to reproduce the linear order as developed by Mukhanov, Feldmann and Brandenberger [8]. The dust serves as a material reference system which we couple dynamically as fields rather than assuming the usual test observers in order to give the Einstein equations (modulo gauge freedom) the interpretation of evolution equations of observable quantities. This leads to in principle observable deviations from the standard formalism which however decay during the cosmological evolution.

In this paper we quantize the algebra of observables constructed in [6]. Actually there is not much to do because that algebra is isomorphic to the Poisson algebra of general relativity plus the standard model on $\mathbb{R} \times \mathcal{S}$ where \mathcal{S} is the dust space manifold. Hence we can take over the kinematical Hilbert space representation that is used in loop quantum gravity (LQG) [9, 10]. For recent reviews on LQG see [11]; for books see [12]. One may object that this representation is less natural here than in usual Dirac-quantized LQG where it is uniquely selected on physical grounds [13, 14], namely one wants to have a unitary representation of the spatial diffeomorphism group of the coordinate manifold \mathcal{X} which is a *gauge group* (passive diffeomorphisms) there. Since all our observables are gauge invariant, we have no diffeomorphism gauge group any longer; hence, that physical selection criterion is absent. However, it is replaced by a different one. It turns out that the physical Hamiltonian has the diffeomorphism group of the dust label space as the *symmetry group*. These diffeomorphisms change our observables, and they are *active diffeomorphisms* since they map between physically distinguishable dust space labels. Thus we may apply the same selection criterion.

Now the interesting remaining question is whether that representation allows us to define the quantized version of the physical Hamiltonian. Maybe not surprisingly, it turns out that the same techniques that allowed us to construct the quantum Hamiltonian constraint [15] and the master constraint [16] in usual Dirac-quantized LQG can be used to define the quantized physical Hamiltonian. This operator is positive, hence symmetric and upon taking its natural Friedrich extension, it becomes self-adjoint. In order to preserve its classical, active, spatial diffeomorphism symmetry it turns out that one has to define it in such a way that it preserves the graph of a spin network function that it acts on. The techniques developed in [17] can now be applied to show, using the semiclassical states introduced in [18], that the physical Hamiltonian has the correct semiclassical limit on sufficiently fine graphs. In fact, in order to get rid of the graph dependence one can use the generalization of LQG to algebraic quantum gravity (AQG) [17]. This casts quantum gravity completely into the framework of (Hamiltonian) lattice gauge theory [19, 20] with one crucial difference. There is no continuum limit to be taken because we are in a background-independent theory with active diffeomorphisms as symmetries.

The attractive feature of this reduced phase space approach is that we no longer need to deal with the constraints: no anomalies can arise, no master constraint needs to be constructed, no physical Hilbert space needs to be derived by complicated group-averaging techniques. We map a conceptually complicated gauge system to the conceptually safe realm of an ordinary dynamical Hamiltonian system. The kinematical results of LQG such as discreteness of spectra of geometric operators now become *physical predictions*. This is a concrete implementation of the programme outlined for the full theory in [21] and generalizes the reduced phase

space techniques recently adopted for the loop quantum cosmology (LQC) truncation of LQG [22–25], which is a toy model for the cosmological sector of LQG, to the full theory.

It ‘remains’ to analyse the physical Hamiltonian in detail since it encodes the complete dynamics of general relativity coupled to the standard model. The following tasks should be addressed in the future.

- (1) *Vacuum and spectral gap.* For a start we note that the physical Hamiltonian does not depend explicitly on an external time parameter. Our Hamiltonian system which dynamically couples geometry and matter is a *conservative* system. This is in contrast to QFT on curved and in particular time-dependent background spacetime metrics where one quantizes matter propagating on an externally given background geometry. The Hamiltonian of that QFT is not preserved and thus even the notion of a ground state or vacuum as a lowest energy eigenstate becomes time dependent which leads to constant particle creation problems, etc [26]. In our approach the notion of a vacuum state would not suffer from those problems. This appears as a conceptual improvement although of course the lowest eigenvalue of the Hamiltonian could be vastly degenerate. Also, the minimum of the spectrum of the Hamiltonian might not lie in its discrete (more precisely, pure point) part so that the ‘ground state(s)’ would not be normalizable.
- (2) *Scattering theory.* With a physical Hamiltonian \mathbf{H} at our disposal we can in principle perform scattering theory, that is, we can compute matrix elements of the time evolution operator $U(\tau) = \exp(i\tau\mathbf{H})$. The analytical evaluation of those matrix elements is of course too difficult but as in ordinary QFT we may use Fermi’s golden rule and expand, for short time intervals τ , the exponential as $U(\tau) = \mathbf{1}_{\mathcal{H}} + i\tau\mathbf{H} + O(\tau)^2$. The matrix elements of \mathbf{H} seem hopeless to compute because it involves square roots of a positive self-adjoint operator for whose precise evaluation we would need the associated projection-valued measure which of course we do not have. However, since in scattering theory initial and final states are excitations over a ground state which we do not know exactly but presumably can approximate by kinematical coherent states, one can invoke the technique developed in [17] to expand the square root of the operator around the square root of its expectation value. We will do this in a future project. Of course there are issues to be resolved such as those of the existence of asymptotic states [27] and how one implements them in our formalism, see e.g. [28] for some basic ideas.
- (3) *Anomalies.* As already mentioned, the Hamiltonian \mathbf{H} has a huge symmetry group of which $\text{Diff}(\mathcal{S})$ is a subgroup and it is easy to implement this symmetry at the quantum level. However, there is another infinite classical, Abelian symmetry group \mathcal{N} which is generated by the Hamiltonian density functions $H(\sigma)$ and in terms of which the Hamiltonian reads $\mathbf{H} = \int_{\mathcal{S}} d^3\sigma H(\sigma)$. Classically one has $\{H(\sigma), H(\sigma')\} = 0$ which of course implies classically that $\{H(\sigma), \mathbf{H}\} = 0$. The Lie algebra of the total classical symmetry group thus consists of infinitesimal active diffeomorphisms and infinitesimal transformations generated by the $H(\sigma)$. The latter form an Abelian Poisson ideal and thus \mathcal{N} is an Abelian invariant subgroup in the total symmetry group which hence is a semidirect product $\mathfrak{G} = \mathcal{N} \rtimes \text{Diff}(\sigma)$. Presumably, in the naive quantization of \mathbf{H} that we consider as a preliminary proposal in this paper, the latter symmetry is explicitly broken, or anomalous although semiclassically it is preserved. In order to reinstall it, one can try to make use of renormalization group techniques associated with the so-called improved or perfect actions [29].
- (4) *Lattice numerical methods.* It transpires that within the framework proposed here many of the conceptual problems of canonical quantum gravity have been solved and the technical tasks have been simplified and reduced to a detailed analysis of the operator \mathbf{H} , of course,

at the price to have introduced additional, albeit unobservable, matter as a material reference system and a possibly only locally (in phase space) description. Since \mathbf{H} is a complicated operator which is formulated in terms of lattice like variables especially in the AQG version, it is natural to use Monte Carlo methods in order to study the operator numerically.

- (5) *QFT on curved spacetimes and standard model.* It is widely accepted that the framework of QFT on curved spacetimes [26] should be an excellent approximation to quantum gravity whenever the metric fluctuations are small. In particular, when the background spacetime is Minkowski, then the standard model must be reproduced. Besides that, one would like to see whether our background-independent lattice theory which is manifestly UV finite and non-perturbative can explore the non-perturbative sector of the standard model such as QCD. Another interesting question is whether our explicitly geometry-matter coupled system can lead to an improved understanding of the Hawking effect due to the possibility of taking care of backreaction effects.
- (6) *Effective action, universality, ambiguities.* Our framework presents a canonical quantization of the field theory underlying the Einstein Hilbert action plus the standard model action. Now computations within perturbative QFT and also string theory suggest that the effective action⁹ for gravity is an extension of the Einstein–Hilbert Lagrangian by higher derivative terms and an often asked question is whether one should not quantize these more general actions. There are several remarks in order.
- (A) The effective action is a complicated, often even non-local, action which takes care of all higher loop diagrams obtained from a simple bare action. It looks like a classical action but it actually encodes all quantum fluctuations. Therefore, it is inappropriate to quantize that classical action anew; it would not produce the same quantum theory as the bare action.
- (B) Still one could just add all possible higher derivative terms from the outset. While one can canonically quantize such theories by the Ostrogradsky formalism, this leads in general to a drastic increase in the number of degrees of freedom [30] due to the appearance of higher time derivatives.
- (C) In the Euclidean formulation of QFT on Minkowski as a path integral one entertains a related (Wilson) notion of effective action as the action that one obtains when integrating out degrees of freedom labelled by (in Fourier space) momenta above a certain energy scale¹⁰. This also produces various higher derivative terms at lower energies as compared to the bare action which is defined at infinite energy. Now the couplings of the bare action also are in principle unknown, however, for many theories that does not matter due to a phenomenon called universality. The couplings of the higher derivative terms depend on the energy scale and a coupling is called relevant, marginal or irrelevant, respectively, if it grows, remains constant or decreases in

⁹ There are several loosely equivalent definitions for the effective action. The notion we mean here is the following. Consider first a renormalizable theory. Given a defining action with a finite number of finite but unknown couplings and masses (parameters) one can perform perturbation theory and discovers, within a given regularization scheme, that the parameters are to be altered by functions of the distance cutoff which diverge in the limit of vanishing cutoff in order to avoid singularities in loop diagrams. If one does this order by order then one ends up with the so-called bare action which produces finite higher loop diagrams to all orders. The effective action is a vehicle that produces the same scattering amplitudes or n -point functions as the bare action but of which one only needs to compute tree diagrams (no loops). The definition for a non-renormalizable theory such as gravity is the same, just that then number of parameters is infinite. In renormalizable theories a finite number of experiments is sufficient to fix the unknown parameters while non-renormalizable theories have no predictive power.

¹⁰ That energy scale has nothing to do with a perturbative cutoff; we are talking here about an already well-defined theory.

the low energy limit. A universal theory is such that all but a finite number of the couplings are irrelevant. One may ask whether one can see universality also in the canonical formalism; however, there are several obstacles in answering this question. First of all, the Euclidean formulation uses a Wick rotation which is only possible for background-dependent theories where the background has a presentation with an analytic dependence on the time coordinate. In quantum gravity the metric becomes an operator; hence, Wick rotation and therefore a Euclidean formulation is not possible. One should therefore define the Wilsonian effective action directly in the Hamiltonian (Lorentzian) formulation, however, that has not been done so far.

It seems to us that in order to make progress on this kind of question one should first try to define a Hamiltonian notion of effective action, see [31] for a possible direction. Then, if the symmetry arguments mentioned under (2.3) are insufficient in order to fix the quantization (discretization) ambiguities in the definition of \mathbf{H} , possibly universality studies may lead to further understanding.

- (7) *Singularity avoidance.* In quantum gravity we expect or want to resolve two types of singularities. First, QFT kind of short-distance singularities which come from the fact that in interacting field theories one has to deal with products of operator-valued distributions. Second, classical general relativity kind of singularities which are simply a feature of the Einstein equations to predict that generically spacetimes are geodesically incomplete. An analytical measure for such spacetime singularities are typically divergences of curvature invariants.

Now as shown in [15], UV-type of singularities are absent at the non-gauge-invariant level, specifically, the quantum constraints are densely defined. In [21] it was discovered, in the context of usual LQG, that expectation values of non-gauge-invariant curvature operators with respect to non-gauge-invariant coherent states that are peaked on a classically singular (FRW) trajectory remain finite as one reaches the singularity, thus backing up the much more spectacular results of [22–25] which are at the level of the physical Hilbert space albeit for a toy model and not the full theory.

While these are encouraging results, they are at the kinematical level only and thus are inconclusive. However, with the technology developed in this paper we can transfer both results *literally and with absolutely no changes* to the physical Hilbert space. As far as the spacetime singularity resolution is concerned, this is still not enough because the coherent states that we are using, while being now physical coherent states, are not adapted to the physical Hamiltonian and thus may spread out under the quantum dynamics generated by $U(\tau)$. In other words, given gauge-invariant initial data $m(0)$ and a coherent state ψ_0 that we prepare at $\tau = 0$ and which is peaked on $m(0)$, it may be that after short time τ the state $U(\tau)\psi_0$ is very different from the state ψ_τ which is peaked on the classical trajectory $\tau \mapsto m(\tau)$. Therefore, in order to come to conclusions one should rather study expectation values with respect to the states $U(\tau)\psi_0$ rather than ψ_τ . In addition, one should try to construct *dynamical* coherent states for which such a spread does not happen. However, this is a difficult task already for the unharmonic oscillator.

The plan of the paper is as follows.

In section 2 we review the essentials of [6, 7] in order to make this paper self-contained. This will lead to the reduced phase space and the classical physical Hamiltonian.

In section 3 we quantize the reduced phase space using methods from LQG and obtain the physical Hilbert space almost for free. Then we implement the physical Hamiltonian on that Hilbert space. We do this both for LQG and the AQG extension.

In section 4 we summarize and conclude.

2. Review of the Brown–Kuchař and relational framework

2.1. Brown–Kuchař Lagrangian

In [1] Brown and Kuchař add the following Lagrangian to the Einstein–Hilbert and standard model Lagrangian¹¹ on the spacetime manifold M :

$$S_D = -\frac{1}{2} \int_M d^4X \sqrt{|\det(g)|} \rho [g^{\mu\nu} U_\mu U_\nu + 1], \quad (2.1)$$

where the one-form U is defined by $U = -dT + W_j dS^j$ and the index j takes values 1, 2, 3 while μ, ν take values 0, 1, 2, 3. The action S_D is a functional of the fields $\rho, g_{\mu\nu}, T, S^j, W_j$. Here T, S^j have dimension of their length, W_j is dimensionless and thus ρ has dimension cm^{-4} .

As shown in [6, 7], in performing the Legendre transformation of (2.1) according to the $3 + 1$ split of $M \cong \mathbb{R} \times \mathcal{X}$ into time and space, one introduces momenta P, P_j, I, I^j conjugate to T, S^j, ρ, W_j , respectively, next to the momenta P^{ab}, p, p_a conjugate to q_{ab}, n, n^a , respectively, where one encounters several primary constraints. Here one has introduced a foliation of M , that is, a one-parameter family of embeddings $t \mapsto X_t : \mathcal{X} \rightarrow \mathcal{X}_t$, where \mathcal{X}_t are the leaves of the foliation and the coordinates on \mathcal{X} are denoted by $x^a, a = 1, 2, 3$. The vector field $\partial_t X_t^\mu = n n^\mu + n^a X_{t,a}^\mu$ can be decomposed into components normal and tangential to the laves where n^μ is the future-oriented normal. The functions n, n^a are the usual lapse and shift functions and $q_{ab} = g_{\mu\nu} X_{,a}^\mu X_{,b}^\nu$ defines the three-metric intrinsic to \mathcal{X} . The aforementioned primary constraints are

$$\begin{aligned} Z := I = 0, \quad Z^j := I^j = 0, \quad Z_j := P_j + P W_j = 0, \\ z := p = 0, \quad z_a := p_a = 0. \end{aligned} \quad (2.2)$$

The stability analysis of these constraints with respect to the corresponding primary Hamiltonian leads to the following secondary constraints:

$$\begin{aligned} c^{\text{tot}} = c + c^D, \quad c^D = \frac{1}{2} \left[\frac{P^2}{\rho \sqrt{\det(q)}} + \rho \sqrt{\det(q)} (1 + q^{ab} U_a U_b) \right] \\ c_a^{\text{tot}} = c_a + c_a^D, \quad c_a^D = P [T_{,a} - W_j S_{,a}^j] \\ \tilde{c} = \frac{n}{2} \left[-\frac{P^2}{\rho^2 \sqrt{\det(q)}} + \sqrt{\det(q)} (1 + q^{ab} U_a U_b) \right] \end{aligned} \quad (2.3)$$

and six more equations which can be solved for the Lagrange multipliers corresponding to constraints Z^j, Z_j and which we do not display here. Here $U_a = -T_{,a} + W_j S_{,a}^j = -c_a^D/P$ and c, c_a^D respectively are the contributions of geometry and standard matter to the usual Hamiltonian and spatial diffeomorphism constraint, respectively.

The stability analysis of the secondary constraints with respect to the primary Hamiltonian which is a linear combination of the constraints (2.2) and the first two constraints in (2.3) reveals that there are no tertiary constraints. Moreover, the classification of the sets of constraints into the first and second-class shows that the constraints $z, z_a, c^{\text{tot}}, c_a^{\text{tot}}$ are first class while, roughly speaking, the pairs $(Z, \tilde{c}), (Z_j, Z^j)$ form second class constraints with non-degenerate matrix

¹¹ Usually Lorentz symmetry breaking is discussed at the Lagrangian level before discussing the phase space and constraint structure of the system. In that sense, our system is perfectly Lorentz invariant (more precisely, spacetime diffeomorphism invariant). The Brown–Kuchar Lagrangian which is our starting point is a bona fide spacetime diffeomorphism-covariant Lagrangian scalar density. With respect to the reduced phase space, which we discuss below, it is physically completely obvious that different observers describe the same physics in different terms (rods and clocks) and one would therefore not expect the reduced action to be ‘label space’ (in our case, dust space) diffeomorphism invariant, see our companion work [6].

formed by their mutual Poisson brackets. Hence, to proceed, one passes to the corresponding Dirac bracket and solves the second-class constraints explicitly by setting

$$I := 0, \quad I^J := 0, \quad W_j := -\frac{P_j}{P}, \quad \rho^2 := \frac{P^2}{\sqrt{\det(q)}}[q^{ab}U_aU_b + 1]. \quad (2.4)$$

Fortunately, the Dirac bracket reduced to the geometry variables q_{ab} , p^{ab} and the remaining matter variables is identical to the original Poisson bracket.

After using (2.4) and solving $z = z_a$ by identifying lapse and shift as Lagrange multiplier functions respectively we are left with the first-class constraints

$$\begin{aligned} c^{\text{tot}} &= c + c^D, & c^D &= -\sqrt{P^2 + q^{ab}c_a^D c_b^D} \\ c_a^{\text{tot}} &= c_a + c_a^D, & c_a^D &= PT_{,a} + P_j S^j_{,a}. \end{aligned} \quad (2.5)$$

In principle we could have chosen the other sign to solve the quadratic equation for ρ in (2.4) but the detailed analysis in [6] reveals that the other choice would produce the Einstein equations with the wrong sign in the limit of vanishing dust fields. In particular one must choose ρ , $P < 0$ so that the additional matter enters with a negative sign into the Hamiltonian constraint. This has the important consequence that $c > 0$ thus enables close to flat space solutions¹².

As far as the physical interpretation of the additional matter is concerned we just mention that its Euler Lagrange equations imply that the vector field $U^\mu = g^{\mu\nu}U_\nu$ is a geodesic in affine parametrization, that the fields W_j , S^j are constant along the geodesic and that the field T defines proper time along each geodesic. It follows that $S^j = \sigma^j = \text{const.}$ labels a geodesic while $T = \tau = \text{const.}$ is an affine parameter along the geodesic. Furthermore, its energy–momentum tensor is that of a perfect fluid with vanishing pressure and negative energy density¹³; hence, it is pressure-free *phantom* dust. It serves as a dynamical, material reference system which also plays the role of a phantom in the literal sense because it is not directly visible in the final picture while leaving its fingerprint on the dynamics.

2.2. Brown–Kuchař mechanism

The observation of Brown and Kuchař was that the constraints (2.5) can be written in a deparametrized form. This holds in more general circumstances, namely whenever we consider scalar fields without potential and mass terms as pointed out in [5]. The observation consists in the fact that the only appearance of T , S^j in c^{tot} is in the form c_a^D . However, this means that using $c_a^{\text{tot}} = 0$ we may write (2.5) in the equivalent form:

$$\begin{aligned} c^{\text{tot}} &= c + c^D, & c^D &= -\sqrt{P^2 + q^{ab}c_a c_b} \\ c_a^{\text{tot}} &= c_a + c_a^D, & c_a^D &= PT_{,a} + P_j S^j_{,a}, \end{aligned} \quad (2.6)$$

¹² As explained in the text, the energy density of the observable matter is supposed to obey the usual energy conditions. This is not in contradiction with the vanishing total Hamiltonian constraint and nowhere vanishing non-positive dust energy conditions since the gravitational contribution to the energy density is indefinite but of course excludes a strictly flat spacetime in the absence of observable matter ('vacuum') which in turn is not in contradiction to the experiment (Minkowski space is only a local approximation to the metric in our universe). The presence of the dust leads to arbitrarily small, nowhere vanishing corrections where 'small' means arbitrarily small in any metric topology. These do not exclude vacuum with respect to observable matter but rather that it is not possible to have both a flat spacetime and no observable matter as already said above. Addressing stability, we are only concerned with the stability of the reduced phase space with respect to the physical Hamiltonian which is manifestly positive and thus renders the system stable.

¹³ We are not violating any energy conditions because we still require that the energy momentum tensor of *observable* (standard) matter plus dust satisfies the energy conditions. In fact, it would be sufficient if the energy conditions are satisfied by the standard matter alone because in the final analysis the dust completely disappears while the equations of motion for observable matter and geometry assume their standard form plus small corrections, see [6, 7].

where equivalent means that in (2.5) and (2.6) the new constraints c' can be expressed in terms of the old ones c as $c'_I = M_I^J c_J$ where M_I^J is a matrix non-singular on the constraint surface defined by the constraint c_I . This means the constraints in equation (2.6) define the same constraint surface and the same gauge-invariant functions.

We can now solve the first equation in (2.6) for P , remembering that $P < 0$ and the second equation for P_j , making the assumption that the matrix $S_{,a}^j$ is everywhere non-degenerate¹⁴ with inverse S_j^a . The result is

$$\begin{aligned}\tilde{c}^{\text{tot}} &= P + h, & h &= +\sqrt{c^2 - q^{ab}c_a c_b} \\ \tilde{c}_j^{\text{tot}} &= P_j + h_j, & h_j &= S_j^a [c_a - h T_{,a}].\end{aligned}\tag{2.7}$$

In solving (2.6) in terms of P we find at an intermediate step that $P^2 = c^2 - q^{ab}c_a c_b$. Hence, while the argument of the square root in (2.7) is not manifestly positive, it is *constrained to be positive*.

Note that the function h is independent of S^j , T while h_j still depends on both. Hence, we have achieved only partial deparametrization. However, this will be sufficient for our purposes. An important consequence is that the constraints in the form (2.7) are mutually Poisson commuting. This follows immediately from an abstract argument¹⁵ [32], although one can also verify this by direct computation [1]. This implies in particular that the $h(x)$ are mutually Poisson commuting while the $h(x)$ do not Poisson commute with the $h_j(y)$ and neither do the $h_j(y)$ among each other.

2.3. Relational framework

2.3.1. General theory. We first consider a general system with first-class constraints C_I with the arbitrary index set \mathcal{I} and later specialize to our situation.

Consider any set of functions T^I on phase space such that the matrix defined by the Poisson bracket entries $M_I^J := \{C_I, T^J\}$ is invertible. Consider the equivalent set of constraints

$$C'_I := \sum_J [M^{-1}]_I^J C_J\tag{2.8}$$

such that $\{C'_I, T^J\} \approx \delta_I^J$ where \approx means = modulo terms that vanish on the constraint surface. Let X_I be the Hamiltonian vector field of C'_I and for any set of real numbers β^I

$$X_\beta := \sum_I \beta^I X_I.\tag{2.9}$$

For any function f on phase space, we set

$$\alpha_\beta(f) := \exp(X_\beta) \cdot f = \sum_{n=0}^{\infty} \frac{1}{n!} X_\beta^n \cdot f.\tag{2.10}$$

¹⁴ This is a classical restriction of the same kind as $\det(q) > 0$. As far as the dynamical stability of the condition is concerned, the expression $\det(S_{,a}^j)$ Poisson commutes with the function h whose observable is the Hamiltonian density of the physical Hamiltonian. Therefore, if the condition $\det(S_{,a}^j) > 0$ is satisfied on the initial hypersurface it remains stable under the dynamics. It is also obviously spatially diffeomorphism invariant. Note that we use the equivalent Hamiltonian constraint $\tilde{c} = P + h$ which is a linear combination of the original constraints with phase space-dependent non-singular coefficients.

¹⁵ The constraints (2.7) are of first class. Hence their Poisson brackets are linear combinations of constraints. Since the constraints are linear in the momenta P, P_j , their Poisson brackets are independent of P, P_j . Therefore, we can evaluate the linear combination of the constraints that appear in the Poisson bracket computation in particular at $P = -h, P_j = -h_j$.

Now let τ^I be another set of real numbers and define

$$O_f(\tau) := [\alpha_\beta(f)]_{\alpha_\beta(T)=\tau}, \quad (2.11)$$

where $\alpha_\beta(T) = \tau$ means $\alpha_\beta(T^I) = \tau^I$ for all I . As one can check, $\alpha_\beta(T^I) \approx T^I + \beta^I$ so that (2.11) is weakly (i.e. on the constraint surface) equivalent to

$$O_f(\tau) := [\alpha_\beta(f)]_{\beta=\tau-T}. \quad (2.12)$$

Note that after equating β with $\tau - T$, the previously phase space independent quantities β become phase space dependent; therefore, it is important in (2.12) to *first* compute the action of X_β with β treated as phase space independent and only *then* to set it equal to $\tau - T$.

The significance of (2.12) lies in the following facts.

- (1) The functions $O_f(\tau)$ are weak Dirac observables with respect to the C_I , that is,

$$\{C_I, O_f(\tau)\} \approx 0. \quad (2.13)$$

This remarkable property is due to the key observation that the X_I weakly commute [3, 4].

- (2) The multi-parameter family of maps $O^\tau : f \mapsto O_f(\tau)$ is a homomorphism from the commutative algebra of functions on phase space to the commutative algebra of weak Dirac observables, both with pointwise multiplication, that is,

$$O_f(\tau) + O_{f'}(\tau) = O_{f+f'}(\tau), \quad O_f(\tau)O_{f'}(\tau) \approx O_{ff'}(\tau). \quad (2.14)$$

The linear relation is obvious; the multiplicative one follows from the fact that

$$\alpha_\beta(ff') = e^{X_\beta} \cdot ff' = e^{X_\beta} \cdot ff' e^{-X_\beta} \cdot 1 = [e^{X_\beta} \cdot f e^{-X_\beta}][e^{X_\beta} f' e^{-X_\beta}], \quad (2.15)$$

where we used the identity

$$[e^{X_\beta} \cdot f e^{-X_\beta}] = \sum_{n=0}^{\infty} \frac{1}{n!} [X_\beta, f]_{(n)} \quad (2.16)$$

and where X_β, f respectively are considered as derivation and multiplication operators respectively on the algebra of functions on phase space so that $[X_\beta, f] = X_\beta \cdot f$. Here $[X, f]_{(0)} = f, [X, f]_{(n+1)} = [X, [X, f]_{(n)}]$.

- (3) The multi-parameter family of maps $O^\tau : f \mapsto O_f(\tau)$ is in fact a Poisson homomorphism with respect to the Dirac bracket $\{.,.\}^*$ defined by the second-class system C_I, T^J , that is,

$$\{O_f(\tau), O_{f'}(\tau)\} \approx \{O_f(\tau), O_{f'}(\tau)\}^* \approx O_{\{f,f'\}^*}(\tau), \quad (2.17)$$

where the Dirac bracket is explicitly given by

$$\{f, f'\}^* = \{f, f'\} - \{f, C_I\} [M^{-1}]_I^J \{T^J, f'\} + \{f', C_I\} [M^{-1}]_I^J \{T^J, f\}. \quad (2.18)$$

Here we have used in the first step that both $O_f(\tau), O_{f'}(\tau)$ have weakly vanishing brackets with the constraints. Relation (2.17) follows from the fact that the map α_β is a Poisson automorphism on the algebra of functions on phase space and the Poisson bracket must be replaced by the Dirac bracket because in evaluating $\{O_f(\tau), O_{f'}(\tau)\}$ we must take care of the fact that $\beta = \tau - T$ is phase space dependent. See [4] for the explicit proof.

The interpretation of $O_f(\tau)$ is that it is a relational observable, namely it is the value of f in the gauge $\beta = T - \tau$.

2.3.2. *Specialization to deparametrized theories.* For deparametrized theories it is possible to find canonical coordinates consisting of two sets of canonical pairs (P^I, T^I) and (q^a, p_a) respectively (where the Poisson brackets between elements of the first and second set vanish) such that the constraints C_I can be rewritten in the equivalent form:

$$C_I = P_I + h_I(q^a, p_a), \quad (2.19)$$

that is, they no longer depend on the variables T^I . This is a very special case and most gauge systems cannot be written in this form. Even with dust general relativity is *a priori* not of that form; however, we will reduce it to that form with an additional manipulation below.

The simplifications that occur are now the following.

(A) We obviously have

$$M_I^J = \{C_I, T^J\} = \delta_I^J; \quad (2.20)$$

therefore, $C'_I = C_I$ and we do not have to invert a complicated matrix.

(B) By the same argument as in the footnote after (2.7) we have $\{C_I, C_J\} = 0$ identically on the full phase space, not only on the constraint surface which of course implies that $\{X_I, X_J\} = 0$; the Hamiltonian vector fields of the constraints are mutually commuting. It also follows that $\{h_I, h_J\} = 0$ and thus $\{C_I, h_J\} = 0$ for all I, J which means that the h_I are already Dirac observables.

These simplifications mean that all the previous weak equalities become strong ones, i.e. identities on the full phase space. The Dirac observable associated with T_I

$$O_{T_I}(\tau) = [\alpha_\beta(T^I)]_{\alpha_\beta(T)=\tau} = \tau^I \quad (2.21)$$

is simply the constant (on phase space) function τ^I . The momenta P_I are already Dirac observables; however, they can be expressed in terms of q^a, p_a via the constraints. Moreover, since O^τ is a homomorphism we have on the constraint surface

$$P_I = O_{P_I}(\tau) = -O_{h_I}(\tau) = -h_I(O_{q^a}(\tau), \quad O_{p^a}(\tau)) =: -H_I. \quad (2.22)$$

In fact we have $h_I = H_I$ because h_I is already a Dirac observable.

The reduced phase space (where the constraints hold and where the gauge transformations have been factored out) is therefore coordinatized by the functions

$$Q^a(\tau) = O_{q^a}(\tau), \quad P_a(\tau) = O_{p_a}(\tau) \quad (2.23)$$

and in what follows we concentrate on functions f which only depend on q^a, p_a . On such functions the Dirac bracket reduces to the Poisson bracket since $\{T_I, f\} = 0$ for all I . Therefore, the reduced map $O^\tau : f \mapsto O_f(\tau)$ is now a multi-parameter Poisson *automorphism* with respect to the Poisson bracket. In particular we note

$$\{P_a(\tau), Q^b(\tau)\} = \{O_{p_a}(\tau), O_{q^a}(\tau)\} = O_{\{p_a, q^b\}}(\tau) = O_{\delta_a^b}(\tau) = \delta_a^b \quad (2.24)$$

which means that the reduced phase space has a very simple symplectic structure in terms of the coordinates $P_a := P_a(0), Q^a := Q^a(0)$ which in fact form a conjugate pair. It is this fact which makes reduced phase space quantization feasible as observed in [4].

It seems that we have trivialized everything. However, this is not the case as we must interpret the τ dependence of our observables. We note first of all that on functions f independent of T^I , P_I formula (2.12) reads explicitly

$$O_f(\tau) = \alpha_\tau(f) = \exp(X_\tau) \cdot f = \sum_{n=0}^{\infty} \frac{1}{n!} X_\tau^n \cdot f, \quad (2.25)$$

where X_τ is the Hamiltonian vector field of the function $H_\tau = (\tau^I - T^I)H_I$. Here we have used that the X_I on f reduce to the Hamiltonian vector field of h_I and since h_I is independent

of P_J we may write $O_f(\tau)$ in the above compact form. It is now a simple exercise to verify that [4]

$$\partial O_f(\tau)/\partial \tau^I = \{H_I, O_f(\tau)\} \quad (2.26)$$

which means that the strongly Abelian group of Poisson automorphisms α_τ is generated by the ‘Hamiltonians’ H_I . Thus, if we interpret the T_I as clocks then we have a multi-fingered time evolution with Hamiltonians H_I .

In quantum theory then one would like to select a suitable one-parameter family by prescribing functions $\tau^I(s)$ in terms of a single parameter such that the associated Hamiltonian is positive and has preferred physical properties.

2.4. The reduced phase space of general relativity with dust

Now we specialize to our situation which is a special case of the general theory. This has been previously done in detail, including proofs, in [5] and was also reviewed in [6]. Here we summarize those results.

As previously mentioned, the Hamiltonian constraints in (2.7) are in deparametrized form; however, the spatial diffeomorphism constraints are not. However, the idea is to exploit the fact that the constraints (2.7) are mutually Poisson commuting so that one can perform the reduction of the phase space in two steps. First we reduce with respect to the spatial diffeomorphism constraint and then with respect to the Hamiltonian constraint. More precisely, consider arbitrary functions β^0, β^j on \mathcal{X} and denote by X_β the Hamiltonian vector field of the function

$$c_\beta^{\text{tot}} := \int_{\mathcal{X}} d^3\sigma \beta^\mu(x) \tilde{c}_\mu^{\text{tot}}(x), \quad (2.27)$$

where we have defined $\tilde{c}_0^{\text{tot}} = \tilde{c}^{\text{tot}}$. Then for arbitrary functions $\tau^0(x) = \tau(x)$, $\tau^j(x) := \sigma^j(x)$ on \mathcal{X} the general formula reads

$$O_f(\tau) = [\alpha_\beta(f)]_{\alpha_\beta(T)=\tau}, \quad \alpha_\beta(f) = \exp(X_\beta) \cdot f, \quad (2.28)$$

where $T^0(x) = T(x)$, $T^j(x) = S^j(x)$. We readily compute that $\alpha_\beta(T^\mu(x)) = T^\mu(x) + \beta^\mu(x)$ so that

$$O_f(\tau) = [\alpha_\beta(f)]_{\beta=\tau-T}. \quad (2.29)$$

Now since $S^j(x)$ Poisson commutes with $\tilde{c}^{\text{tot}}(y)$, we may rewrite (2.29) in the form

$$O_f(\tau) = [\alpha_{\beta^0}([\alpha_{\tilde{\beta}}(f)])]_{\tilde{\beta}=\tilde{\sigma}-\tilde{S}}]_{\beta^0=\tau-T}. \quad (2.30)$$

It turns out that one can compute the inner argument of (2.30) rather explicitly with an immediate physical interpretation for judicious choices of the functions $\sigma^j(x)$. Namely, for any scalar function f built from of T, P, q_{ab}, p^{ab} and the matter of the standard model, one finds explicitly that for *constant* functions σ^j

$$[\alpha_{\tilde{\beta}}(f(x))]_{\tilde{\beta}=\tilde{\sigma}-\tilde{S}} = f(x)_{\tilde{S}(x)=\sigma}. \quad (2.31)$$

In other words, whatever the value of x at which the function f is evaluated, (2.31) evaluates it at the point x_σ^a at which $S^j(x)$ assumes the value σ^j . Since we have assumed that S_a^j is everywhere invertible and thus defines a diffeomorphism between \mathcal{X} and the range of S^j which is the *dust space* \mathcal{S} , the value x_σ is unique. Formula (2.31) is proved explicitly in [6] and will not be repeated here. Thus, (2.31) takes a simple form if we choose as f one of the following functions on \mathcal{S} :

$$\tilde{T} := T, \quad \tilde{P} = \frac{P}{J}, \quad \tilde{q}_{jk} := q_{ab} S_j^a S_k^b, \quad \tilde{p}^{jk} := \frac{p^{ab} S_a^j S_b^k}{J}, \quad (2.32)$$

where

$$J := \det(\partial S / \partial x) \quad (2.33)$$

as well as

$$\begin{aligned} \tilde{a}_j^I &:= a_b^I S_j^b, & \tilde{e}_I^j &:= \frac{e_I^a S_a^j}{J}, & \tilde{\psi}_{\alpha I} &:= \psi_{\alpha I}, \\ \tilde{\bar{\psi}}_{\alpha I} &:= \bar{\psi}_{\alpha I}, & \tilde{\phi}_I &:= \phi_I, & \tilde{\pi}^I &:= \frac{\pi^I}{J} \end{aligned} \quad (2.34)$$

for connections a_b^I , electric fields e_I^a , fermions $\psi_{\alpha I}$, $\bar{\psi}_{\alpha I}$ and Higgs fields ϕ_I with conjugate momentum π^I of the standard model where I labels a basis in the Lie algebra of the appropriate gauge group; see [15] for the canonical formulation of the standard model coupled to gravity including appropriate background independent Hilbert space representations.

It is clear that the evaluation of the functions (2.32) and (2.34) at x_σ is nothing else than the pull back of the corresponding fields to \mathcal{S} under the inverse of the diffeomorphism $S^j : \mathcal{X} \rightarrow \mathcal{S}$. We will denote the corresponding tensor fields on \mathcal{S} as in (2.32) and (2.34). Note that while these are scalars on \mathcal{X} they are tensor densities of the same weight on \mathcal{S} as they have¹⁶ on \mathcal{X} . In [1, 6] it is shown that one can arrive at the spatially diffeomorphism-invariant functions (2.32) and (2.34) also by symplectic reduction with respect to the spatial diffeomorphism constraint which is an alternative proof of the fact that canonical pairs without tilde on \mathcal{X} are mapped to canonical pairs on \mathcal{S} . For instance

$$\{\tilde{p}^{jk}(\sigma), \tilde{q}_{mn}(\sigma')\} = \kappa \delta_{(m}^j \delta_{n)}^k \delta(\sigma, \sigma'), \quad (2.35)$$

where $\kappa = 16\pi G_{\text{Newton}}$. This also shows that it is sufficient to consider constant σ^j rather than arbitrary functions.

Returning to (2.30) we see that it remains to compute

$$O_f(\tau, \sigma) := [\alpha_{\beta^0}(f(\sigma))]_{\beta^0 = \tau - T}, \quad (2.36)$$

where f is now an arbitrary function of the spatially diffeomorphism-invariant functions (2.32) and (2.34). Now we can use the simplified theory of section 2.3.2 because \tilde{c}^{tot} is written in deparametrized form, i.e. it does not involve T , S^j any longer. Actually, formula (2.36) would be awkward for non-constant functions τ because it depends on

$$c_\tau^{\text{tot}} = \int_{\mathcal{X}} d^3x (\tau - T)(x) \tilde{c}^{\text{tot}}(x), \quad (2.37)$$

which is expressed on the space \mathcal{X} rather than dust space \mathcal{S} . However, for constant τ (2.37) is the integral of a density of weight 1 and can then be written in the form

$$c_\tau^{\text{tot}} = \int_{\mathcal{S}} d^3\sigma (\tau - \tilde{T})(\sigma) [\tilde{P} + \tilde{h}](\sigma), \quad (2.38)$$

¹⁶ This statement sounds contradictory because of the following subtlety. We have e.g. the three quantities $P(x)$, $\tilde{P}(x) = P(x)/J(x)$, $\tilde{P}(\sigma) = \tilde{P}(x_\sigma)$. On \mathcal{X} , $P(x)$ is a scalar density while $\tilde{P}(x)$ is a scalar. Pulling back $P(x)$ to $\mathcal{S} = S(\mathcal{X})$ by the diffeomorphism $\sigma \mapsto S^{-1}(\sigma)$ results in $\tilde{P}(\sigma)$. But pulling back $\tilde{P}(x)$ back to \mathcal{S} results in the *same* quantity $\tilde{P}(\sigma)$. Since a diffeomorphism does not change the density weight, we would get the contradiction that $\tilde{P}(\sigma)$ has both density weights 0 and 1 on \mathcal{S} . The resolution of the puzzle is that what determines the density weight of $P(x)$ on \mathcal{X} is its transformation behaviour under canonical transformations generated by the total spatial diffeomorphism constraint $c_a^{\text{tot}} = c_a^D + c_a$, where c_a^D , c_a are the dust and non-dust contributions respectively. After the reduction of c_a^{tot} , what determines the density weight of $\tilde{P}(\sigma)$ on \mathcal{S} is its transformation behaviour under $([c_a + PT_{,a}]S_j^a/J)(x_\sigma) = \tilde{c}_j(\sigma) + \tilde{P}(\sigma)\tilde{T}_{,j}(\sigma)$ and this shows that $\tilde{P}(\sigma)$ has density weight 1.

where

$$\begin{aligned}\tilde{h}(\sigma) &= \sqrt{\tilde{c}(\sigma)^2 - \tilde{q}^{jk}(\sigma)\tilde{c}_j(\sigma)\tilde{c}_k(\sigma)} \\ \tilde{c}(\sigma) &= \frac{c}{J}(x_\sigma) \\ \tilde{c}_j(\sigma) &= \frac{c_a S_j^a}{J}(x_\sigma).\end{aligned}\quad (2.39)$$

Note that e.g. \tilde{c} is just the pull back of c and that one simply has to replace every tensor without tilde by their pulled back image with tilde. Thus, constant τ is uniquely selected by the requirement that c_τ^{tot} is spatially diffeomorphism invariant.

It follows now from section 2.3.2 that

$$O_f(\tau, \sigma) = \sum_{n=0}^{\infty} \frac{1}{n!} \{H_\tau, f(\sigma)\}_{(n)}, \quad H_\tau = \int_S d^3\sigma [\tau - T](\sigma) \tilde{h}(\sigma) \quad (2.40)$$

and that

$$\frac{d}{d\tau} O_f(\sigma, \tau) = \{\mathbf{H}, O_f(\sigma, \tau)\}, \quad \mathbf{H} = \int_S d^3\sigma \tilde{h}(\sigma). \quad (2.41)$$

Since the $h(x)$ are mutually Poisson commuting, it follows that also the $\tilde{h}(\sigma)$ are mutually Poisson commuting so that

$$H(\sigma, \tau) := \alpha_{\beta^0}(\tilde{h}(\sigma))_{\beta^0=\tau-T} = \tilde{h}(\sigma) =: H(\sigma) \quad (2.42)$$

is independent of τ and already a Dirac observable.

Note that the physical Hamiltonian \mathbf{H} is positive. It enjoys the following symmetries. Since it is an integral over a density of weight 1 it is invariant under diffeomorphisms of S . Note that S is a label space for geodesics and not a coordinate manifold; hence, in contrast to the passive diffeomorphism group $\text{Diff}(\mathcal{X})$, the group $\text{Diff}(S)$ are *active* diffeomorphisms. In particular, it follows that

$$\{\mathbf{H}, \tilde{c}_j(\sigma)\} = 0, \quad (2.43)$$

which also is a consequence of having chosen constant τ , in which case the physical Hamiltonian has a maximal amount of symmetry. Had we not chosen constant τ then the physical Hamiltonian *would not be a Dirac observable*.

This also implies that

$$\{\mathbf{H}, C_j(\sigma)\} = 0, \quad C(\sigma, \tau) := \alpha_{\beta^0}(\tilde{c}_j(\sigma))_{\beta^0=\tau-T} =: C_j(\sigma) \quad (2.44)$$

is actually independent of τ , although $\tilde{c}_j \neq C_j$. Note that

$$H(\sigma) = \sqrt{C(\sigma, \tau)^2 - Q^{jk}(\sigma, \tau)C_j(\sigma)C_k(\sigma)}, \quad C(\sigma, \tau) := \alpha_{\beta^0}(\tilde{c}(\sigma))_{\beta^0=\tau-T}. \quad (2.45)$$

The second symmetry of \mathbf{H} is of course that

$$\{\mathbf{H}, H(\sigma)\} = 0. \quad (2.46)$$

Let us write for some scalar and vector test functions f, u^j respectively

$$H(f) := \int_S d^3\sigma f(\sigma) H(\sigma), \quad C(u) := \int_S d^3\sigma u^j(\sigma) C_j(\sigma); \quad (2.47)$$

then,

$$\begin{aligned}\{C(u), C(u')\} &= -\kappa C(\{u, u'\}) \\ \{C(u), H(f')\} &= -\kappa H(u[f']) \\ \{H(f), H(f')\} &= 0\end{aligned}\quad (2.48)$$

which shows that the symmetry generators generate an honest Lie algebra \mathfrak{g} in contrast to the Dirac algebra underlying GR as was pointed out already in [1] and further examined in [33]. That Lie algebra has a subalgebra generated by the $C(u)$ and an Abelian ideal generated by the $H(f)$; hence, it is not semisimple. The corresponding Lie group $\mathfrak{G} = \mathcal{N} \rtimes \text{Diff}(\mathcal{S})$ is therefore the semidirect product of the Abelian invariant subgroup \mathcal{N} to which the $H(f)$ exponentiate and the active diffeomorphism group of dust space.

2.5. Physical interpretation and comparison with unreduced formalism

The symmetry algebra \mathfrak{g} and the associated conservation laws play a crucial role in showing [6] that the equations of motion for the canonical pairs of true degrees of freedom

$$(Q_{jk}, P^{jk}); (A_j^I, E_I^j); (\Psi_{\alpha I}, \bar{\Psi}_{\alpha I}); (\Phi_I, \Pi^I) \quad (2.49)$$

which are the images of the canonical pairs

$$(\tilde{q}_{jk}, \tilde{p}^{jk}); (\tilde{a}_j^I, \tilde{e}_I^j); (\tilde{\psi}_{\alpha I}, \tilde{\bar{\psi}}_{\alpha I}); (\tilde{\phi}_I, \tilde{\pi}^I) \quad (2.50)$$

under $\alpha_{\beta^0}(\cdot)_{\beta^0=\tau-T}$ at $\tau = 0$ assume the standard form that they have in general relativity without dust [34], with two important modifications. First, in usual general relativity without dust the equations of motion generated by the canonical Hamiltonian $h(n, \vec{n}) = c(n) + \bar{c}(\vec{n})$ which is a linear combination of the smeared Hamiltonian constraint $c(n) = \int_{\mathcal{X}} d^3x n c$ and spatial diffeomorphism constraint $\bar{c}(\vec{n}) = \int_{\mathcal{X}} d^3x n^a c_a$ involve arbitrary lapse and shift functions n, n^a on \mathcal{X} which are independent of phase space. However, in our formalism lapse and shift functions become dynamical functions¹⁷ on \mathcal{S} , namely $N = C/H$ and $N^j = -Q^{jk}C_k/H$. Second, without dust we still have constraints $c = c_a = 0$ while we have energy–momentum conservation laws $H = \epsilon, C_j = -\epsilon_j$ where ϵ, ϵ_j are arbitrary functions on \mathcal{S} independent of τ . This turns dynamical lapse and shift into a function of $Q^{jk}, \epsilon_j/\epsilon$. The functions ϵ, ϵ_j express the influence of the dust on the other variables and are the price to pay for having a manifestly gauge-invariant formalism rather than assuming non-dynamical test observers that turn geometry and matter into observable quantities.

This concludes the classical analysis and the review of [6].

3. Reduced phase space quantization of general relativity

3.1. Hilbert space representation

Let us summarize the result of the previous section. By using the relational formalism we can explicitly compute the reduced phase space of general relativity with dust. It is *identical* to the unreduced phase space without dust with proper identification of \mathcal{X} with \mathcal{S} and of the gauge-invariant canonical pairs (2.49) with the gauge-variant canonical pairs

$$(q_{ab}, p^{ab}); (a_b^I, e_I^b); (\psi_{\alpha I}, \bar{\psi}_{\alpha I}); (\phi_I, \pi^I) \quad (3.1)$$

of geometry and standard matter. The constraints have disappeared, they have been solved and reduced. Instead of a linear combination of constraints on the gauge-variant phase space coordinatized by (3.1) which generates gauge transformations, there is a physical Hamiltonian (2.41) which generates physical time evolution on the gauge-invariant phase coordinatized by (2.49). From the classical point of view one should now simply solve those equations in physically interesting situations. In [6, 7] we have done this in the context of cosmological

¹⁷ This is similar in spirit to [35] where one replaces lapse and shift test fields by hand by phase space-dependent functions, carefully chosen (via Witten spinor techniques that enter the proof of the gravitational positive energy theorem) so that the resulting Hamiltonian is positive, at least on shell.

perturbation theory [6, 7] which is written in manifestly gauge-invariant form. This not only reproduces the standard results [8] but will also allow us to investigate higher order perturbation theory without running into problems with gauge invariance.

In the quantum theory we are looking for representations of the Poisson *-algebra generated by (2.49) which supports a quantized version of the Hamiltonian \mathbf{H} . The selection of appropriate representations will be guided by the symmetry group \mathfrak{G} unveiled in the previous section. First of all, since we consider fermionic matter we are forced to work with tetrads rather four-metrics. We use the second-order formalism as displayed in [15] (that is, we write the Einstein–Hilbert Lagrangian in terms of the spin connection of the tetrad which involves second-order derivatives rather than using the first-order Palatini formalism) in order to avoid torsion. This means that we formulate the geometry phase space in terms of $su(2)$ connections and canonically conjugate fields (A_I^J, E_I^J) rather than in terms of the ADM variables Q_{jk}, P^{jk} where I is an $su(2)$ index. This casts the geometry sector of the phase space into an $SU(2)$ Yang–Mills theory description. The price to pay is that there is an additional Gauss constraint on the phase space (which has been reduced only with respect to the Hamiltonian and spatial diffeomorphism constraint) given by

$$G_I := \partial_j E_I^j + \epsilon_{JK} A_J^j E_K^j + \text{fermion terms} \quad (3.2)$$

just as for the matter Yang–Mills variables (we assume that the Cartan Killing metric is always δ_{JK} by appropriate normalization of the Lie algebra basis).

The gauge field language suggests to formulate the theory in terms of holonomies along one-dimensional paths and electric fluxes through two-dimensional surfaces, just as in unreduced LQG. There one has a uniqueness result [13, 14] which says that cyclic representations of the holonomy-flux algebra which implement a unitary representation of the spatial diffeomorphism gauge group $\text{Diff}(\mathcal{X})$ are unique and are unitarily equivalent to the Ashtekar–Isham–Lewandowski representation [9, 10]. In our case we do not have a diffeomorphism gauge group but rather a diffeomorphism symmetry group $\text{Diff}(\mathcal{X})$ of the physical Hamiltonian \mathbf{H} . This is physical input enough to also insist on cyclic $\text{Diff}(\mathcal{S})$ covariant representations and correspondingly we can copy the uniqueness result.

Thus we simply choose the background-independent and active diffeomorphism-covariant Hilbert space representation of LQG used extensively in [15] and we ask whether that representation supports a quantum operator corresponding to \mathbf{H} .

3.2. Subtleties with the Gauss constraints

Before we analyse this question in detail, we should mention a subtlety. When one rewrites the geometry and standard matter contributions c, c_a to the total Hamiltonian and spatial diffeomorphism constraint in terms of the gauge theory variables, one can do this in G invariant form (where G is the compact gauge group underlying the corresponding Yang–Mills theory) only by introducing terms proportional to the Gauss constraint, see e.g. [12]. For instance, the contribution to the spatial diffeomorphism constraint of a Yang–Mills field on the unreduced phase space is given by

$$c_a^{YM} = f_{ab}^I e_I^b - a_a^I g_I^{YM} = \tilde{c}_a^{YM} - a_a^I g_I^{YM}, \quad (3.3)$$

where $f_{ab}^I = 2\partial_{[a} a_{b]}^I + \epsilon_{JK} a_a^J a_b^K$ is the curvature of the connection a_a^I and ϵ_{JK} are the structure constants of the corresponding Lie algebra. The function (3.3) really generates Yang–Mills gauge transformations; however, it is itself of course not Yang–Mills gauge invariant due to the term proportional to the Gauss constraint

$$g_I^{YM} = \partial_a e_I^a + \epsilon_{JK} a_a^J e_K^a. \quad (3.4)$$

Likewise, the geometry contribution c^{geo} to c contains a term proportional to g_I^{geo} [12] (however, c^{YM} does not). As far as the definition of the complete constraint surface is concerned, one can drop the various Gauss law contributions to c , c_a since we impose the Gauss laws independently anyway. This gives an equivalent set of constraints which is such that c , c_a are manifestly invariant under Yang–Mills type of Gauss transformations. However, now the algebra of the c^{tot} , c_a^{tot} only closes up to a term proportional to the various Gauss laws.

The question is now whether this spoils the argument that the constraints in the form (2.7) are mutually Poisson commuting. In fact, we only can conclude that their Poisson brackets are proportional to \tilde{c}^{tot} , \tilde{c}_a^{tot} and the various g_I^{YM} while they must not depend on the dust momenta P , P_j . This means that their Poisson brackets are proportional to a Yang–Mills gauge-invariant linear combination of Gauss constraints. Hence, indeed the constraints \tilde{c}^{tot} , \tilde{c}_a^{tot} are Abelian only on the constraint surface of the Gauss constraints.

This poses the question which consequence this has for the formalism developed in the previous section. First of all, all relations that we have written there remain valid modulo terms proportional to the Gauss constraints. Second, the physical Hamiltonian is manifestly Yang–Mills gauge invariant, manifestly $\text{Diff}(\mathcal{X})$ invariant and invariant modulo the Gauss constraints under \mathcal{N} .

The strategy that we adopt is the following. In the presence of gauge fields we actually work with the non-Gauss-invariant contributions to the spatial diffeomorphism constraints as in (3.3) and with the non-Gauss-invariant contribution to c^{geo} such that algebra of Hamiltonian and spatial diffeomorphism constraints closes without involvement of the Gauss constraints. This makes the analysis of the previous section go through without modifications at the price that the physical Hamiltonian is not Gauss invariant. When we quantize it turns out that one can actually solve the various Gauss constraints explicitly by Dirac constraint quantization. That is, the Hilbert space can be projected to the Gauss-invariant subspace which has an explicitly known orthonormal basis given by the Gauss-invariant spin network functions (and their analogue for the gauge group of the standard model). Therefore, on the Gauss-invariant Hilbert space one can actually replace the C_j^{YM} by \tilde{C}_j^{YM} because the correction term proportional to the Gauss constraint vanishes on the Gauss-invariant Hilbert space (upon appropriate ordering of the Gauss constraint operator to the right so that no commutator terms arise). Thus C_j is replaced by its Gauss-invariant analogue and similarly one can replace C by its Gauss-invariant analog so that H and \mathbf{H} become manifestly Gauss-invariant operators and \mathbf{H} should have the symmetry group \mathfrak{G} as well.

An alternative route would be to also reduce the phase space with respect to the Gauss constraints, possibly using the framework of [36] and references therein.

3.3. Quantum Hamiltonian

3.3.1. Sign issues and strategy. Before we go into details we must worry about yet another issue. As we have seen in the classical analysis, the expression $H^2 = C^2 - Q^{JK} C_J C_K$ is constrained to be non-negative. Actually we have seen this only for $c^2 - q^{ab} c_a c_b$ but as we showed

$$(C^2 - Q^{jk} C_j C_k)(\sigma) = ([c^2 - q^{ab} c_a c_b]/J)(x_\sigma) \quad (3.5)$$

and $J > 0$ by assumption (we have imposed $J \neq 0$ everywhere; hence either $J > 0$ everywhere or $J < 0$ everywhere by continuity and we choose the first option). However, on the full, reduced phase space $C^2 - Q^{jk} C_J C_K$ maybe indefinite. In the quantum theory we therefore should derive, roughly speaking, a self-adjoint operator (valued distribution) for $H^2(\sigma)$ and restrict the spectral resolution of the Hilbert space to the positive spectrum

part. This has to be done for *every* σ . This may be impossible because the corresponding spectral conditions could be incompatible. However, as already pointed out by Brown and Kuchař [1], if we indeed manage to quantize $H^2(\sigma)$ in such a way that they are mutually commuting¹⁸, then the corresponding spectral projections commute and the above requirement is consistent. Unfortunately, it might not only be difficult to achieve commutativity of the operators corresponding to the various $H^2(\sigma)$, but it will also be difficult to compute the corresponding projection-valued measures.

Therefore, as a first step, in this paper we adopt the following strategy. Classically, in the interesting part of the phase space we have $C^2 - Q^{jk}C_jC_k \geq 0$. Therefore, on this part of the phase space we have trivially $C^2 - Q^{jk}C_jC_k = |C^2 - Q^{jk}C_jC_k|$. Hence, on that part of the phase space we have the identity

$$H = \sqrt{|C^2 - Q^{jk}C_jC_k|} = \sqrt{\frac{1}{2}([C^2 - Q^{jk}C_jC_k] + |C^2 - Q^{jk}C_jC_k|)}. \quad (3.6)$$

The virtue of this rewriting is that both expressions, which are identical on the physically interesting piece of the phase space, can be extended to the full phase space without becoming imaginary. In the second version, the function actually vanishes on the unphysical part of the phase space. In either form, the square root now makes sense in the quantum theory because its argument is now a non-negative expression.

We remark that a discussion of similar sign issues and whether one should allow states in the quantum theory, which violate the classical positivity of $H^2(\sigma)$ which is enforced by a constraint of the form $P^2 - H^2 = 0$ and where H^2 is not manifestly positive while P^2 surely is, can be found for instance in [37]. There the authors argue that one should allow negative energy states because otherwise one would exclude the tunnelling effects into the classically not allowed regions which, as we know from quantum mechanical experiments, do happen. What happens mathematically is that in the operator constraint method (Dirac approach), one quantizes both P and H^2 as self-adjoint operators on the *kinematical* Hilbert space and then solves the quantum constraint. The elements of the corresponding physical Hilbert space may have support in the classically not allowed region of the configuration space (where they typically decay rather than oscillate) so that the expectation value of $H^2 = P^2$ becomes negative. This is possible only because the operator corresponding to P , while being a quantum Dirac observable, does not descend to a self-adjoint operator on the physical Hilbert space. In a *strict* reduced phase space quantization, one would have to restrict the physical Hilbert space to states which have support only in the classically allowed region of the phase space and this may well be the physically correct procedure. However, for the moment, as we do not yet have sufficient control over the spectrum of H^2 , we comply with the conclusion of [37] and do not make any restriction on the physical Hilbert space.

Thus, in this paper we therefore propose to quantize the first version of (3.6) which is a classically valid starting point¹⁹. We then adopt a naive quantization strategy and are able to construct a well-defined Hamiltonian operator. That quantization not necessarily has the property that the quantized versions of the $H^2(\sigma)$ are mutually commuting and therefore the operator constructed in this paper should only be considered as a preliminary step. However, that operator has the following three properties. It is manifestly Gauss invariant, manifestly $\text{Diff}(\mathcal{S})$ covariant and has the correct classical limit in the sense of expectation values and fluctuations with respect to coherent states. However, it maybe anomalous with respect to

¹⁸ More precisely, one has to demand that the projection-valued measures E_σ for the $H^2(\sigma)$ mutually commute in order to avoid domain questions. Note that the Poisson commutativity of the $H(\sigma)$ implies the Poisson commutativity of the $H^2(\sigma)$ and vice versa.

¹⁹ A similar strategy was adopted for the quantization of the volume in LQG. Classically we have $\det(q) = \det(E) > 0$ but in order to give meaning to $\sqrt{\det(q)}$ in the quantum theory we must start from $\sqrt{|\det(E)|}$.

the group \mathcal{N} . In fact, the absence of that anomaly would be mathematically equivalent to showing that the Dirac algebra of general relativity is implemented non-anomalously. We stress, however, that the gauge symmetries of general relativity have been exactly taken care of in the reduced phase space approach. We are talking here about a symmetry group and not a gauge group. To break a local gauge group is usually physically unacceptable especially in renormalizable theories where the corresponding Ward identities find their way into the renormalization theorems. However, it may or may not be acceptable that a physical symmetry is (spontaneously, explicitly, etc) broken. For instance, the explicit breaking of the axial vector current Ward identity in QED, also called the ABJ anomaly, is experimentally verified.

In the lack of a physical justification for why the \mathcal{N} symmetry should be broken, we view that potential anomaly as an indication that the quantization of the present paper has to be improved. In fact, since we are effectively working with a background-independent lattice gauge theory, it is useful to adopt strategies from lattice gauge theory in order to restore symmetries on the lattice that are broken in a naive quantization. It turns out that in fortunate cases one can restore the symmetry by making the operator quasi-non-local. That is, in addition to next-neighbour interactions one has to consider next-to-next-neighbour interactions, etc which makes the action non-local; however, the coefficients of those additional interactions decay exponentially with the lattice distance. See e.g. [29] and references therein.

We consider the completion of this step as a future research programme. In the course of that analysis we might even be able to fix the quantization (discretization) ambiguities, i.e. the coefficients in front of the various n th neighbour contributions.

With this cautionary remarks out of the way, we can now consider a naive quantization of the Hamiltonian which is strongly guided by analogous techniques developed for the Hamiltonian and Master constraint of unreduced LQG [15, 16] so that these constructions are also helpful in the present reduced phase space approach.

3.3.2. Naive quantization.

Classical regularization. We begin with some classical considerations and we focus on the gravitational contributions to C , C_j and for C only on the Euclidean piece. For the matter contributions and the Lorentzian piece the necessary, completely analogous manipulations can be found in [17]. Consider a partition \mathcal{P} of \mathcal{S} into cubes \square so that

$$\mathbf{H} = \sum_{\square \in \mathcal{P}} \int_{\square} d^3\sigma \sqrt{|C^2 - Q^{jk}C_jC_k|}(\sigma). \quad (3.7)$$

Let $V_0(\square)$ be the coordinate volume of \square in any coordinate system and let $\sigma(\square)$ be some coordinate point inside \square with respect to the same coordinate system. Then we can write (3.7) as the limit, in which the partition becomes the continuum, of the following Riemann sum approximation of the above integral:

$$\mathbf{H} = \lim_{\mathcal{P} \rightarrow \mathcal{S}} \sum_{\square \in \mathcal{P}} V_0(\square) \sqrt{|C^2 - Q^{jk}C_jC_k|}(\sigma(\square)). \quad (3.8)$$

Using the classical identities

$$Q^{jk} = \frac{E_j^I E_k^J \delta^{IJ}}{\det(Q)}, \quad E_I^j = \sqrt{\det(Q)} e_I^j, \quad (3.9)$$

where $I, J, \dots = 1, 2, 3$ label a basis $\tau_I = -i\sigma_I$ (where σ_I denote the Pauli matrices) in $su(2)$ and e_I^j denotes the triad, it is not difficult to verify that

$$C^2 = [\text{Tr}(B)]^2, \quad Q^{jk}C_jC_k = [\text{Tr}(B\tau_I)]^2/4 =: C_I^2. \quad (3.10)$$

Here we have introduced the magnetic field $B_I^j = \frac{1}{2}\epsilon^{jkl}F_{kl}^I$ and have set $B^j = B_I^j\tau_I$, $e_j = e_j^I\tau_I$, $B = B^j e_j$ where e_j^I denotes the cotriad. We may further write

$$\mathbf{H} = \lim_{\mathcal{P} \rightarrow \mathcal{S}} \sum_{\square \in \mathcal{S}} \sqrt{|C(\square)^2 - \delta^{IJ}C_I(\square)C_J(\square)|}, \quad (3.11)$$

where

$$C(\square) := \int_{\square} d^3\sigma C(\sigma), \quad C_I(\square) := \int_{\square} d^3\sigma C_I(\sigma). \quad (3.12)$$

The strategy is now to quantize the objects (3.12) and to define

$$\hat{\mathbf{H}} := \lim_{\mathcal{P} \rightarrow \mathcal{S}} \sum_{\square \in \mathcal{S}} \sqrt{|\hat{C}(\square)^\dagger \hat{C}(\square) - \delta^{IJ} \hat{C}_I(\square)^\dagger \hat{C}_J(\square)|} \quad (3.13)$$

provided the limit exists. For $C(\square)$ this has been done in the literature [15, 16] and we follow the same strategy here. In fact we can treat both C , C_I in a unified way. We have with $\tau_0 := 1_2$

$$\int_{\square} d^3\sigma \text{Tr}(B\tau_\mu) = \int_{\square} \text{Tr}(F \wedge e\tau_\mu) = \frac{1}{\kappa} \int_{\square} \text{Tr}(F \wedge \{V(\square), A\}\tau_\mu), \quad (3.14)$$

where

$$V(\square) = \int_{\square} d^3\sigma \sqrt{\det(Q)} \quad (3.15)$$

is the *physical* volume of \square . Actually there is a sign of $\det(e)$ involved in (3.15) but this is cancelled in the squares that appear in (3.11).

The virtue of writing (3.14) in this form is that (3.15) can be quantized on the LQG Hilbert space; hence, one replaces the Poisson bracket by the commutator divided by $i\hbar$. Thus one is left with the quantization of the connection A and its curvature F . This is the source of many ambiguities already in unreduced LQG because A , F do not exist as operators, what exists are holonomies along paths and loops respectively which can be used in order to approximate A , F respectively. However, while classically there are infinitely many ways to do this with the same continuum limit, in the quantum theory each choice leads to a different regularized operator in unreduced LQG, see [15]. In unreduced LQG one can still argue that most of the uncountably infinite number of choices are gauge-related under the spatial diffeomorphism group and in fact spatial diffeomorphism invariance is used in order to carry out the limit $\mathcal{P} \rightarrow \mathcal{X}$ in a specific operator topology [11, 15]. However, in reduced LQG the spatial diffeomorphism group is no longer a gauge group; it is a symmetry group of the dynamics. Therefore, these two arguments are no longer available and therefore the ambiguity issue appears to be much worse in reduced LQG. This is the first indication that calls for the AQG generalization.

In the next paragraph we will discuss to what extent those ambiguities persist in reduced LQG, in the paragraph after that we use the AQG reformulation.

Reduced LQG: embedded graphs. We want to define the Hamiltonian operator $\hat{\mathbf{H}}$ on the Gauss-invariant Hilbert space of LQG which we will denote by \mathcal{H} . This Hilbert space has an orthonormal basis consisting of spin network functions $T_{\gamma,j,I}$ where γ is a (semianalytic) graph embedded into \mathcal{S} , $j = \{j_e\}_{e \in E(\gamma)}$ is a collection of non-vanishing spin quantum numbers (one for each edge) and $I = \{I_v\}_{v \in V(\gamma)}$ is a collection of Gauss-invariant intertwiners (one for each vertex). There is a unitary action of the active diffeomorphisms on this Hilbert space defined by

$$U(\varphi)T_{\gamma,j,I} = T_{\varphi(\gamma),j,I}. \quad (3.16)$$

In unreduced LQG the diffeomorphisms are considered as gauge transformations and therefore the states (3.16) are all gauge related. In the reduced formalism of this paper the states of the form are physically distinguishable. Therefore, it does not make physical sense to construct diffeomorphism-invariant distributions which sometimes are used in the construction of Hamiltonian or master constraint operators as already pointed out.

This last point has crucial bearing on the quantization strategy. If we want to preserve the classical symmetry of the Hamiltonian operator under diffeomorphisms, then this operator must be quantized in a *graph non-changing way* [38] on \mathcal{H} . By this is meant the following. Let \mathcal{H}^γ be the closed linear span of spin network states over γ . Then \mathcal{H} is the direct sum of the \mathcal{H}^γ , that is,

$$\mathcal{H} = \bigoplus_\gamma \mathcal{H}^\gamma \tag{3.17}$$

which shows that the *physical* Hilbert space \mathcal{H} is non-separable. This is an important difference with non-reduced LQG where the physical Hilbert space can be made separable if one extends the spatial passive diffeomorphism group beyond the differentiable category [39]. This is a second indication that one should possibly leave the strict realm of (reduced) LQG and pass to another framework where non-separable Hilbert spaces can be avoided. This calls for the AQG extension [17] which we discuss in the subsequent paragraph.

In any case, graph non-changing in the sense of [38] now means that the operator $\widehat{\mathbf{H}}$ should preserve *each* \mathcal{H}^γ *separately!* This appears as if we had to assume an infinite number of conservation laws that the classical theory did not have which is a second point to worry about and presents a third motivation to switch to the AQG extension of LQG. However, let us see how far we can get within the usual formalism. To that end, we use the notion of a minimal loop originally introduced in [28] and also used to some extent in [16].

Definition 3.1. *Given a graph γ , consider a vertex $v \in V(\gamma)$ and a pair $e, e' \in E(\gamma)$ of distinct edges incident at v and with outgoing orientation. A loop $\alpha_{\gamma,v,e,e'}$ in γ starting at v along e and ending at v along $(e')^{-1}$ is said to be minimal provided that there exists no other loop in γ with the same properties and fewer edges traversed. The set of minimal loops in γ with data v, e, e' will be denoted by $L_{\gamma,v,e,e'}$.*

Note that the definition is background independent and diffeomorphism covariant.

Given a graph γ and a vertex $v \in V(\gamma)$ we define for $\mu = 0, 1, 2, 3$

$$\begin{aligned} \widehat{C}_{\mu,\gamma,v} := & \frac{1}{\ell_P^2 |T_v(\gamma)|} \sum_{(e_1, e_2, e_3) \in T_v(\gamma)} \epsilon^{IJK} \frac{1}{|L_{\gamma,v,e_I,e_J}|} \sum_{\alpha \in L_{\gamma,v,e_I,e_J}} \\ & \times \text{Tr}(\tau_\mu A(\alpha) A(e_K) [A(e_K)^{-1}, \widehat{V}_{\gamma,v}]), \end{aligned} \tag{3.18}$$

where $T_v(\gamma)$ is the set of ordered triples (i.e. order matters) of distinct edges of γ incident at v taken with outgoing orientation, $A(p)$ denotes the holonomy of the connection A along a path p and

$$\widehat{V}_{\gamma,v} = \ell_P^3 \sqrt{\left| \frac{1}{48} \sum_{e_1, e_2, e_3 \in T_v(\gamma)} \sigma(e_1, e_2, e_3) \epsilon^{LMN} X_{e_1}^L X_{e_2}^M X_{e_3}^N \right|} \tag{3.19}$$

is the projection of the volume operator [40] to²⁰ \mathcal{H}^γ for an infinitesimal neighbourhood of v . Here $\sigma_v(e_1, e_2, e_3)$ is the sign of the determinant of the matrix formed by the tangents of those

²⁰ The alternative volume operator [41] was ruled out in [42] as inconsistent with the classical Poisson bracket identity (3.14). In unreduced LQG one could still say that the volume operator and the Poisson bracket identity are relations among non-observable objects but this is no longer true in reduced LQG as considered here and hence the objection [42] must be taken seriously.

three edges at v and X_e denotes the right invariant vector field on $SU(2)$ associated with the copy of $SU(2)$ coordinatized by $A(e)$.

Finally we set

$$\hat{\mathbf{H}}_\gamma := \sum_{v \in V(\gamma)} \sqrt{\left| P_\gamma \left[\hat{C}_{\gamma,v}^\dagger \hat{C}_{\gamma,v} - \frac{1}{4} \hat{C}_{I,\gamma,v}^\dagger \hat{C}_{I,\gamma,v} \right] P_\gamma \right|}, \quad (3.20)$$

where $P_\gamma : \mathcal{H} \rightarrow \mathcal{H}^\gamma$ denotes the orthogonal projection and makes sure that $\hat{\mathbf{H}}$ is not graph changing, i.e. preserves \mathcal{H}^γ . The dagger operation is that on \mathcal{H} for the operator defined in (3.18) using that entries of holonomies matrices are just multiplication operators and that $\hat{V}_{\gamma,v}$ is self-adjoint.

The operator $\hat{\mathbf{H}}$ is now simply

$$\hat{\mathbf{H}} = \oplus_\gamma \hat{\mathbf{H}}_\gamma. \quad (3.21)$$

It is easy to check that it is diffeomorphism invariant:

$$U(\varphi) \hat{\mathbf{H}} U(\varphi)^{-1} = \hat{\mathbf{H}} \quad (3.22)$$

for all φ . Moreover, it is manifestly Gauss invariant. One may ask what happened to the limit $\mathcal{P} \rightarrow \mathcal{S}$. The answer is that we *define* the operator $\hat{\mathbf{H}}$ as in (3.22) and just check that its expectation values with respect to suitable semiclassical states reproduce the classical function $\hat{\mathbf{H}}$. Such states in particular must use sufficiently large and fine graphs in order to fill out \mathcal{S} . What the operator does on small graphs is irrelevant from the point of view of the classical limit.

With the methods of [17] one should be able to verify that on such graphs the semiclassical limit of the operator is correct. However, that calculation is of course graph dependent.

Reduced AQG: abstract (algebraic) graphs. One of the motivations for the AQG extension of LQG is the graph dependence of the semiclassical calculations. The other is the necessarily graph-preserving feature of diffeomorphism-invariant operators which appears to say that there is an uncountably infinite number of conservation laws that the classical theory does not have. Finally, the non-separability of the Hilbert space \mathcal{H} even if \mathcal{S} is compact without boundary is disturbing. In a sense, to use all graphs is a vast over-counting of degrees of freedom, at least from the classical perspective. To see this, suppose for simplicity that \mathcal{S} is topologically \mathbb{R}^3 (or an open neighbourhood thereof) and thus can be covered by a single coordinate system. Consider piecewise analytic paths which consist of segments along the coordinate axes. Likewise, consider piecewise analytic surfaces which are composed out of segments of coordinate planes. It is clear that the holonomies along those kind of paths and fluxes through that kind of surfaces separates the points of the reduced phase space.

It is true that also in canonical QFT the quantum configuration space is always a distributional enlargement of the classical configuration space. However, there it is never the case that the label set of those fields is uncountable. For instance, in free scalar field theory on Minkowski space the quantum configuration space consists of Schwartz distributions rather than smooth functions. The label set of the fields consists of test functions of rapid decrease which are dense in the Hilbert space of square integrable functions on \mathbb{R}^3 and there exists a countable orthonormal basis of that Hilbert space consisting of Schwarz functions (e.g. Hermite functions times a Gaussian). Thus, the quantum fields are tested by a countable set of test functions and an orthonormal basis in the QFT Hilbert space is labelled by that countable set. In LQG on the other hand the quantum connections are tested by all graphs which is an uncountable set and states over different graphs are orthogonal. So the situation is completely different which seems to be the price of having a diffeomorphism covariant theory [13, 14].

One could of course restrict the labels to those mentioned above but these would not be preserved by diffeomorphisms. It is true that the diffeomorphic image of a coordinate segment can be approximated by coordinate segments; however, the length of say a rotated segment when approximated by a staircase will differ largely from the original length. The same happens for areas of surfaces. The only chance that this does not happen is for observables that are integrals over three-dimensional regions as pointed out in [43].

To make progress on those issues, we therefore will restrict attention to operators that come from integrals over regions of \mathcal{S} such as the volume operator or the Hamiltonian operator. This does not mean that one cannot construct length and volume operators, one just has to define them in an indirect way. In fact, we will only consider quantizing functions which are $\text{Diff}(\mathcal{S})$ invariant. The motivation for doing this is that in physics we do not specify spatial regions by considering a 3D subset R of \mathcal{S} and define, say, a $\text{Diff}(\mathcal{X})$ -invariant volume functions (i.e. a function invariant under *passive* diffeomorphism starting from the unreduced formalism) by

$$V(R) := \int_{\mathcal{X}} d^3x \chi_R(S(x)) \sqrt{\det(q)}(x), \quad (3.23)$$

where χ_R denotes the characteristic function of the set R . Rather we use *observable* matter for doing this. To be sure, (3.23) is $\text{Diff}(\mathcal{X})$ invariant, being the integral of a scalar density over all of \mathcal{X} . In fact, we can pull back this expression to \mathcal{S} and obtain

$$V(R) = \int_{\mathcal{S}} d^3\sigma \chi_R(\sigma) \sqrt{\det(\tilde{q})}(\sigma) = \int_R d^3\sigma \sqrt{\det(\tilde{q})}(\sigma), \quad (3.24)$$

where $\tilde{q} = (S^{-1})^* q$ which would be a mathematically natural object to consider in the reduced theory (after further applying $\alpha_{\beta^0}(\cdot)_{\beta^0=\tau-T}$). It is, however, not $\text{Diff}(\mathcal{S})$ invariant. However, from the point of view of observation one would rather like to consider an object of the form

$$V(I) := \int_{\mathcal{X}} d^3x \chi_I(\phi(x)) \sqrt{\det(q)}(x), \quad (3.25)$$

where I is a subset of the real axis and ϕ is a scalar field. Note that (3.25) is $\text{Diff}(\mathcal{X})$ invariant but it is not a Dirac observable yet. It measures the volume of the subset of \mathcal{X} in which ϕ has a range in I . Now we apply the map O^τ and immediately obtain

$$O_{V(I)}(\tau, \sigma) := \int_{\mathcal{S}} d^3\sigma \chi_I(\Phi(\tau, \sigma)) \sqrt{\det(Q)}(\tau, \sigma), \quad (3.26)$$

where $\Phi(\tau, \sigma) = O_{\phi(x)}(\tau, \sigma)$ (for any x) is the Dirac observable associated with ϕ . Curiously, (3.26) is a Dirac observable and it is $\text{Diff}(\mathcal{S})$ invariant. It measures the physical volume of the region in \mathcal{S} where the physical scalar field Φ ranges in I . The argument shows that $\text{Diff}(\mathcal{S})$ -invariant observables *naturally* arise from the point of the unreduced theory and from operational considerations.

Having motivated to consider only $\text{Diff}(\mathcal{S})$ -invariant observables we are now ready to consider the AQG framework. Since for such observables the coordinate system plays no role we generalize from embedded to non-embedded graphs and the above argument shows that infinite cubic algebraic graphs should be sufficient although a generalization to arbitrary countable algebraic graphs as sketched in [17] would be desirable²¹. In this paper we will just consider the cubic graph for simplicity.

²¹ The idea would be to consider the most general such graph which is the maximal algebraic graph. This is an algebraic graph with a countably infinite number of vertices and with a countably infinite number of edges between each pair of vertices including loops. This generalizes the notion of a complete graph which is a graph in which a single edge connects each pair of vertices.

At the algebraic level the notion of $\text{Diff}(S)$ and even of S itself is meaningless. Note that in AQG the infinite algebraic graph is a fundamental object. This fundamental graph does not change. What does change under the dynamics are subgraphs of the algebraic graph. In other words, subgraphs of the fundamental algebraic graph are not preserved under the quantum dynamics²². The definition of $\hat{\mathbf{H}}$ in AQG is much simpler and no longer involves the projection operators P_γ , so we do not have the awkward conservation laws any longer. In fact, there is no dependence on any algebraic subgraph whatsoever. In complete analogy²³ to [17] it is given by the following list of formulae:

$$\hat{C}_{\mu,v} := \frac{1}{24\ell_P^2} \sum_{s_1, s_2, s_3 = \pm 1} s_1 s_2 s_3 \epsilon^{I_1 I_2 I_3} \text{Tr}(\tau_\mu A(\alpha_{v; I_1 s_1, I_2 s_2}) A(e_{v; I_3 s_3}) [A(e_{v; I_3 s_3})^{-1}, \hat{V}_v]), \quad (3.27)$$

where $e_{v; I_s}$ is the edge beginning at v in the positive ($s = 1$) or negative ($s = -1$) I direction and $\alpha_{v; I_s, J_{s'}}$ is the unique minimal loop in the cubic algebraic graph with data $v, e_{v; I_s}, e_{v; J_{s'}}$. Formula (3.27) is actually the specialization of (3.18). The operator \hat{V}_v is the algebraic volume operator

$$\hat{V}_v = \ell_P^3 \sqrt{\left| \frac{1}{48} \sum_{s_1, s_2, s_3 = \pm 1} s_1 s_2 s_3 \epsilon^{IJK} \epsilon_{LMN} X_{e_{v; I s_1}}^L X_{e_{v; J s_2}}^M X_{e_{v; K s_3}}^N \right|}. \quad (3.28)$$

Finally

$$\hat{\mathbf{H}} := \sum_v \sqrt{\left| \hat{C}_{0,v}^\dagger \hat{C}_{0,v} - \frac{1}{4} \hat{C}_{I,v}^\dagger \hat{C}_{I,v} \right|}, \quad (3.29)$$

where the sum is over all of the infinite number of vertices of the algebraic graph. The operator (3.29) is manifestly Gauss invariant.

The Hilbert space of AQG is the infinite tensor product (ITP) of Hilbert spaces $L_2(SU(2), d\mu_H)$, one for each edge of the graph (this can be generalized to defining different ITPs that come into play when constructing Gauss-invariant states). This Hilbert space is not separable but it is a direct sum of separable Hilbert spaces which assume a Fock-like structure and which are preserved²⁴ by $\hat{\mathbf{H}}$. As far as the symmetry group \mathfrak{G} is concerned, at the algebraic level for instance we no longer have spatial diffeomorphisms. However, we have its algebraic version which consists of the following. Consider the master constraint-like functional

$$M := \int_S d^3\sigma \frac{aH^2 + bQ^{jk} C_j C_k}{\sqrt{\det(Q)}}, \quad (3.30)$$

where $b > a > 0$ are any real numbers. Then a classical function F is invariant with respect to transformations generated by H, C_j respectively if and only if $\{F, \{F, M\}\}_{M=0} = 0$. The functional (3.30) can be quantized on the AQG Hilbert space by literally the same techniques

²² This bears some resemblance with the models for emergent gravity considered in [44] although the dynamics of those models not obviously models the dynamics of \mathbf{H} .

²³ In [17] we considered the extended Master constraint which involves, in the language of this paper, $[C^2 + Q^{jk} C_j C_k] / \sqrt{\det(Q)}$ rather than $\sqrt{|C^2 - Q^{jk} C_j C_k|}$. Hence apart from the sign in front of $Q^{jk} C_j C_k$ we only need to change the power of the volume operator from $V_v^{1/2}$ in [17] to V_v here.

²⁴ We do not know whether $\hat{\mathbf{H}}$ is densely defined on all of the ITP. However, if it is defined on a single vector in a given separable sector then it is densely defined on the entire sector. Now each separable sector of the ITP is labelled by a cyclic vector Ω which is explicitly known. Now $\hat{\mathbf{H}}$ is defined on a given Ω if and only if it is densely defined on the corresponding sector. Hence, for each Ω we just have to perform this test and we simply remove the sectors from the ITP on which $\hat{\mathbf{H}}$ is not densely defined, if any, since they are unphysical. $\hat{\mathbf{H}}$ is certainly densely defined on the sectors built from semiclassical Ω ; hence, the surviving part of the ITP certainly includes all the semiclassical states.

as in [17]. Thus, we have the possibility of analysing the anomaly issue with respect to \mathfrak{G} at the algebraic level as well.

Finally, we can compute the expectation value of $\hat{\mathbf{H}}$ with respect to semiclassical states as in [17] and to zeroth order in \hbar we should find that the classical value is reproduced with small fluctuations. As for the master constraint, the really astonishing fact is that $\hat{\mathbf{H}}$ is a finite operator without renormalization, thanks to our manifestly background-independent formulation. Namely, at the fundamental quantum level the operator algebra is labelled by a single, countably infinite abstract, that is non-embedded, graph Γ . There is no such thing as a lattice distance which would need a background metric. However, the semiclassical states depend on a differential manifold \mathcal{X} , an embedding Y of the algebraic graph Γ into \mathcal{X} , a cell complex $Y(\Gamma)^*$ dual to $Y(\Gamma)$ as well as a point (A_0, E_0) in the classical reduced phase space. Thus, the semiclassical states make contact to the usual (reduced) LQG formulation which in particular uses an at least topological manifold \mathcal{X} . Hence AQG describes all topologies simultaneously. The point is now that, since Γ is an infinite graph, the embedding of Γ can be as fine as we wish, with respect to the spatial geometry described by E_0 even if \mathcal{X} is not compact²⁵. The expectation values of our operators such as $\hat{\mathbf{H}}$ will now give, to zeroth order in \hbar , a Riemann sum approximation of the desired continuum integral $\hat{\mathbf{H}}$ as in (3.14) in terms of holonomies along edges of the embedded graph and the volume of the cubes in the dual-cell complex. The better that a Riemann sum will approximate the integral, the finer the embedding. It is in this sense that in (3.29) no continuum limit has to be performed.

4. Summary and outlook

As compared to the master constraint programme [16], the present framework has the advantage that the master constraint and its solutions are not needed. We directly consider a representation of the gauge-invariant phase space and its Hamiltonian. Celebrated results of unreduced LQG such as the discreteness of the spectrum of kinematical geometric operators [40, 41, 45, 46] which is not granted to survive when passing to the physical Hilbert space [47, 48] in the usual Dirac constraint quantization now becomes a physical prediction if the curves, surfaces and regions that one measures length, area and volume of are labelled by dust space. The Gauss-invariant [49] kinematical coherent states [18] of unreduced LQG now become *physical* coherent states.

However, the physical Hilbert space of reduced LQG is non-separable which appears to be a vast over-counting of quantum degrees of freedom. Passing to AQG means to switch from embedded to non-embedded graphs and thus removes the over-counting. Since for spatially diffeomorphism-invariant operators (on dust space) such as the Hamiltonian $\hat{\mathbf{H}}$ or any other operationally interesting observable (which does not refer directly to the dust label space) the embedding of a graph is immaterial, we can consider the AQG reformulation as an economic description of reduced LQG in the sense that diffeomorphism-related embeddings would lead to isomorphic sectors superselected by this kind of observables. The additional advantage of AQG is that it does not require a topological manifold and that it is free from complications that have to do with graph preservation.

The challenge of the present framework is to implement the (algebraic version of) the symmetry group \mathfrak{G} in the definition of $\hat{\mathbf{H}}$ which will require tools from lattice gauge theory. The final AQG version of the reduced phase space is in any case very similar to Hamiltonian lattice gauge theory with the important difference that no continuum limit has to be taken

²⁵ In the compact case the embedding necessarily has accumulation points but we can choose our states not to be excited on edges that are mapped under the embedding into a suitably small neighbourhood of every accumulation point.

which is why the theory is UV finite. Another important question is how one can understand from the complicated, non-perturbative Hamiltonian \widehat{H} the significance of the standard model Hamiltonian on Minkowski space. The answer to this question must lie in the construction of a minimum energy eigenstate of \widehat{H} which is simultaneously a minimal uncertainty state Ω for all the observables and which is peaked around flat vacuum (no excitations of *observable* matter) spacetime. Presumably, if one studies matter excitations of Ω and considers matrix elements of \widehat{H} in such states, then the resulting matrix elements can be considered as the matrix elements of an effective matter Hamiltonian on Minkowski space which should be close to the Hamiltonian of the standard model on Minkowski space. This expectation is supported by the analysis of [6, 7] which shows that the equations of motion of the gauge-invariant geometry and matter degrees of freedom perturbed around a homogeneous and isotropic (FRW) solution are described effectively by the usual Hamiltonian on a FRW background expanded to second order in the perturbations. Of course, this is only a classical argument. See [28] for more details about the quantum aspects of this idea. We leave this and the research projects mentioned in the introduction for future analysis.

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