Singularities and Quantum Gravity

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Abstract. Although there is general agreement that a removal of classical gravitational singularities is not only a crucial conceptual test of any approach to quantum gravity but also a prerequisite for any fundamental theory, the precise criteria for non-singular behavior are often unclear or controversial. Often, only special types of singularities such as the curvature singularities found in isotropic cosmological models are discussed and it is far from clear what this implies for the very general singularities that arise according to the singularity theorems of general relativity. In these lectures we present an overview of the current status of singularities in classical and quantum gravity, starting with a review and interpretation of the classical singularity theorems. This suggests possible routes for quantum gravity to evade the devastating conclusion of the theorems by different means, including modified dynamics or modified geometrical structures underlying quantum gravity. The latter is most clearly present in canonical quantizations which are discussed in more detail. Finally, the results are used to propose a general scheme of singularity removal, quantum hyperbolicity, to show cases where it is realized and to derive intuitive semiclassical pictures of cosmological bounces.

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1. OVERVIEW

Physical theories are always idealizations without which the complexity of nature would be too great to fathom. Theoretical physics is, mostly very successfully, based on assumptions needed to formulate equations, find solutions and use them to describe, explain and further investigate physical phenomena.

Sometimes, however, these assumptions may not be general enough for all purposes. When they are violated, the theory breaks down which mathematically appears as the development of singularities. An example is given by the use of continuous fields rather than discrete atomic structures in condensed matter physics. When fields vary too strongly on small length scales, such as in shock waves, singularities can occur in continuous field equations even though the basic, discrete physical description remains valid. Usually, deviations between solutions and observations increase before a mathematical singularity is reached. It is then clear that the approximate description can no longer be trusted beyond a certain point. But observations are not always available in such regimes where singularities are approached and an interpretation of mathematical singularities becomes more difficult. This is the case especially for gravity where observations of strong field regimes are lacking.

Singularities in general relativity therefore play a special and dual role. First, the classical importance of singularities can be questioned since there are always assumptions behind special solutions or general theorems leading to singularities. But classical singularities in general relativity also provide an excellent chance to derive implications for the structure of space-time described by general relativity. When the theory breaks down, lessons for space-time structure result which can be especially important for the development of quantum gravity possibly replacing general relativity around classical singularities.

We will first review the classical singularity theorems and sketch their main idea of proof. This will allow us to see which assumptions enter the theorems and what their main conclusions are. These theorems, rather than special singular solutions, define the singularity problem of general relativity. Their statements provide the measuring rod which any proposal for singularity resolution has to be compared with.

The following section will deal with potential examples for singularity resolution which have been proposed in
Quantum gravity, mostly in string theory and in canonical quantizations. The examples are not intended to be complete but to indicate the general types of ideas that have been put forward. (See also [1] for a summary talk.) Here, quantum hyperbolicity will be formulated as a general principle and it will be shown to require characteristic properties of quantum gravity to be realized.

Our specific formulation of the principle is worded in the language of canonical quantum gravity which is described in a subsequent section. We start with an explanation of the difficulties encountered in the first attempts of Wheeler–DeWitt quantizations, and show how their resolution naturally leads to loop quantum gravity. Quantum geometry and quantum dynamics in this framework are then discussed at length, as they provide the main pillars for any attempt to address the fate of classical singularities.

In this framework, loop quantum cosmology has led to explicit constructions of dynamical laws from which non-singular behavior can be derived in several models. This is where the principle of quantum hyperbolicity is currently realized without counterexamples. Loop quantum cosmology thus provides the most general scheme of singularity removal available at present, and it can be used for explicit scenarios.

In most cases, however, the basic description around a classical singularity requires deep quantum regimes which do not lend themselves easily to intuitive interpretations. It can thus be helpful to develop effective descriptions which capture some quantum effects but are otherwise based on classical concepts. This is available in semiclassical bounce pictures which provide examples of how singularities can be avoided through bounces in certain regimes. It also provides the basis for perturbation theory to compute phenomenological and potentially observable effects of metric modes and other fields traveling through a classical singularity.

Although ideas in all five lectures are closely related, the text of any section can be read largely independently of the others.

2. CLASSICAL SINGULARITIES

General relativity describes the gravitational field as a consequence of the space-time structure determined in terms of the metric tensor as a solution to Einstein’s equation $G_{ab} = 8\pi GT_{ab}$ sourced by the energy-momentum tensor $T_{ab}$ coupled through the gravitational constant $G$. In component form, these are coupled, non-linear partial differential equations of second order for the space-time metric $g_{ab}$. Unlike other fundamental field theories, they are generally covariant under arbitrary changes of space-time coordinates which shows that there is no background space and time on which fields are defined. This implies gauge symmetries for the space-time metric.

Gauge theories in general are more systematically analyzed in a canonical formulation where one uses fields and their momenta rather than fields and their time derivatives. One is thus breaking up space-time tensors into spatial and time components which hides the underlying general covariance. To introduce this in general relativity, one foliates space-time into a family of spatial slices $\Sigma_t$ parameterized by an arbitrary time coordinate $t$. The space-time metric adapted to this foliation can be written as

$$ds^2 = -N^2 dt^2 + q_{ab}(dx^a + N^a dt)(dx^b + N^b dt)\quad (1)$$

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2 We will mainly follow the notation used in [4]. In particular, we adopt the abstract index notation where objects such as $T_{ab}$ denote tensors rather than single components in specific coordinates. Expressions only true in certain coordinates are indicated with greek indices. We do not use different types of indices for space-time tensors and spatial tensors; it is rather clear from the context whether an object refers to a space-time or spatial manifold. Note also that $N$ and $N^a$ denote different objects, a function in the first and a vector field in the second case, although traditionally the same letter is used.
with the spatial metric \( q_{ab} \), on \( \Sigma \), the lapse function \( N \) and the spatial shift vector \( N^a \). The components are all functions of spatial coordinates on \( \Sigma \) as well as time \( t \). When inserted in Einstein’s equation, evolution equations in \( t \),

\[
q_{ab} = \frac{16\pi GN}{\sqrt{\det q}} (2p_{ab} - p^c q_{ab}) + 2D(aN_b) \tag{2}
\]

and

\[
\dot{p}_{ab} = -\frac{N}{16\pi G} \frac{\sqrt{\det q}}{(3)R^{ab} - \frac{1}{2}(3)R q^{ab} + \frac{8\pi G N}{\sqrt{\det q}} q^{ab}(p^d p_{cd} - \frac{1}{2}(p^c)^2) - \frac{32\pi GN}{\sqrt{\det q}} (p^ac p_c^b - \frac{1}{2} p^b p^c) \quad \tag{3}
\]

result from the space-space components written in first order form for the spatial metric \( q_{ab} \) and its momentum \( p^{ab} = \frac{\sqrt{q}(K^{ab} - K_c^{ab})}{16\pi G} \) which is related to extrinsic curvature \( K_{ab} = (2N)^{-1}(q_{ab} - D_a N_b - D_b N_a) \) of the spatial slices in space-time. In all equations, \( D_a \) denotes the spatial covariant derivative compatible with \( q_{ab} \), and \((3)R_{ab}\) its Ricci tensor. It is clear from those equations that the components \( N \) and \( N^a \) do occur in the evolution equations of \( q_{ab} \), but are themselves unrestricted (except by the condition that \( q \) must be a Lorentzian metric).

### 2.1. Initial value problem

We thus obtain an initial value problem only once lapse function \( N \) and shift vector \( N^a \) have been specified throughout space-time as a gauge choice. (See [\[3\]] for a discussion of the types of initial value problems realized in general relativity.) Their equations can be interpreted as determining the manifold structure of space-time, which is most clearly seen when using the gauge source function \( \Gamma^a = g^{\nu\lambda} \Gamma^\nu_{\nu\lambda} \). When conditions are imposed by fixing \( \Gamma^a \), a gauge is determined. Notice that the Christoffel symbol \( \Gamma^\nu_{\nu\lambda} \) does not form a tensorial object, which we mark here by using the tilde on one index, and thus fixing its values even to zero restricts the choice of coordinate systems.

Thus, fixing \( \Gamma^a \) implies conditions on the gauge functions \( N \) and \( N^a \). Through the usual relation

\[
\Gamma^\nu_{\nu\lambda} = \frac{1}{2} g^{\mu\nu} (\partial_\lambda g_{\mu\rho} + \partial_\rho g_{\nu\lambda} - \partial_\nu g_{\rho\lambda})
\]

between \( \Gamma^\nu_{\nu\lambda} \) and \( g_{ab} \), one has, for instance,

\[
\partial_t N - N^a \partial_a N = N^2 (K_a^a - n^a \Gamma_a)
\]

which is an identity between \( \Gamma^a \) and the canonical metric components if \( \Gamma^a \) is kept free. (The vector field \( n^a \) is the unit normal vector to the spatial slices.) If \( \Gamma^a \) is prescribed as a gauge choice, however, the equation becomes an evolution equation for \( N \) in this chosen gauge.

Moreover, we have

\[
\Gamma^\nu = g^{\mu\nu} \Gamma^\mu_{\mu\lambda} \delta^\nu_\lambda = -\frac{1}{2} \nabla^\nu \nabla_\lambda \delta^\nu_\lambda = -\nabla_\mu \nabla^\mu \chi^\nu
\]  

such that prescribing \( \Gamma^a \) poses “evolution” equations for space-time coordinates \( x^\mu \). A common choice is the harmonic gauge \( \Gamma^a = 0 \) where coordinates are harmonic functions. Once coordinates on an initial spatial slice are chosen, space-time coordinates are determined as a solution of (5) by fixing the gauge source function.

The space-time manifold as a topological set equipped with an atlas of coordinate charts is thus, to some degree, part of the solution as a consequence of general covariance. This is entirely different from other field theories for fields on a given background (metric) manifold as they are used for the remaining fundamental forces. This does not only give rise to complicated conceptual and technical issues when a quantization is attempted, as we will see later, but also to new physical features already present in the classical theory which are sometimes disturbing. We are able to derive properties of space and time themselves, and about their ends. Although not much is known about general solutions of Einstein’s non-linear partial differential equations, there is one general feature common to most realistic solutions of general relativity: Space-time cannot be extended arbitrarily but develops boundaries where the classical theory breaks down.
2.2. Singularities

Since it is difficult to determine solutions or even asymptotic properties in general, a useful idea is to employ test particles as probes of possible space-time boundaries. One thus studies how test objects behave in a given solution to Einstein’s equation and whether their motion, as described by the classical theory, has to stop at a certain point. If this occurs, the failure to move the test object further can only be attributed to a boundary of space-time itself since no interactions are included which could destroy the object. Quite surprisingly, this procedure allows far-reaching conclusions with only the slightest input from Einstein’s equation [4, 5].

The precise criterion for a space-time singularity in this sense is geodesic incompleteness: space-time is singular if a geodesic, i.e. a word-line of a freely falling test object, exists which is not complete and not extendible. Thus, a curve \( e: \mathcal{I} \to M \) exists whose tangent vector satisfies \( \omega^a \nabla_a \dot{e}^b = 0 \), i.e. it is a piece of an affinely parameterized geodesic defined on a proper subset \( \mathcal{I} \subset \mathbb{R} \) which cannot be extended to be defined on a larger subset \( \mathcal{I} \subset \mathcal{I} \). As the trajectories of freely falling particles, geodesics describe test objects subject only to the gravitational force.

Before we sketch the main proof of a singularity theorem, we collect the typical assumptions and properties used:

- Positive energy conditions, translated to positive curvature through Einstein’s equation, imply focusing of families of geodesics and thus self-intersections and caustics.
- Topological properties of space-time such as global hyperbolicity or spatial non-compactness then allow one to relate properties of geodesic families to space-time properties.
- Appropriate initial configurations select physical situations, such as an everywhere expanding/contracting spatial slice (cosmology) or the existence of a trapped surface (black holes) where, with the preceding two assumptions, singularities are bound to occur.

The proof we sketch here demonstrates the importance of all these assumptions and illustrates how they could potentially be circumvented. To be specific, we focus on singularities as they occur in black holes, requiring the existence of a trapped surface as an initial condition. More details and different types of theorems can be found in [5, 6].

2.2.1. Trapped surfaces

A trapped surface is a compact, 2-dimensional smooth space-like submanifold \( T \subset M \) such that the families of outgoing as well as ingoing future-pointing null normal geodesics are contracting [7]. A geodesic family is defined by specifying a transversal vector field on a submanifold which uniquely determines a family of geodesic curves through each point of the submanifold in a direction given by the vector field at that point. For a compact 2-surface, we can use the inward pointing and outward pointing null normals as those vector fields, defining the ingoing and outgoing null geodesic families. As shown in Fig. 2, the ingoing family of normal geodesics is usually contracting in the sense that its cross-section area decreases, but conversely one intuitively expects the outgoing family to be expanding. A trapped surface requires even the outgoing family to be contracting and thus occurs only under special circumstances.

To define expansion and contraction of families of null geodesics formally, we use their tangent vector field \( k^a \). Then, \( \text{expansion} \) is defined as \( \theta := \nabla_a k^a \). (This is similar to non-relativistic fluid dynamics where the divergence of a velocity field gives the expansion of fluid volume elements.) Similarly, one can use the tensor \( B_{ab} = \nabla_b k_a \) to introduce...
where we used the Leibniz rule, the geodesic equation and the relation
and in Cartesian coordinates of Minkowski space we have using the commutation of coordinate derivatives,

Thus, if a family of geodesics is non-rotating,

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generators define a family of null geodesics. The null tangent vector field is

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and in Cartesian coordinates of Minkowski space we have $B_{\mu\nu} = \partial_\nu k_\mu$ simply in terms of partial derivatives. Taking the trace, one obtains $\theta = 2\text{sgn}(t)/r$ which diverges at the tip of the cone where the null geodesics intersect and form a caustic.

The relation between self-intersections of geodesic families and the divergence of their expansion is general: Take a geodesic family which initially fills all of space-time, i.e. which emanates transversally from a 3-dimensional submanifold. We can thus define three independent vector fields $\kappa^a$ of the 3-dimensional submanifold in addition to the null tangent vector field $\omega_\nu$, which introduces the Riemann curvature tensor $R_{abc}^{\ d}$.

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using the commutation of coordinate derivatives, $[k, \kappa]^a = k^b \nabla_b \kappa^a - \kappa^b \nabla_b k^a = 0$. Then indeed, expansion

diverges when $\kappa^a$ becomes degenerate

From the geodesic deviation equation (6) we obtain the Raychaudhuri equation as its trace:

Thus, if a family of geodesics is non-rotating which means $\omega_{ab} = 0$ and curvature is non-negative as a consequence of energy conditions (such as the null energy condition $T_{ab} k^a k^b \geq 0$ for all null vectors $k^a$) and Einstein’s equation

FIGURE 3. Light cone in Minkowski space.

shear $\sigma_{ab}$ as its symmetric, trace-free part and rotation $\omega_{ab}$ as its anti-symmetric part (paying due attention to the fact that $k^a$ is null in the precise definition which we are not going to need here). These tensors are subject to evolution equations along $\sigma^a$, following from the geodesic equation:

$k^c \nabla_c B_{ab} = k^c (\nabla_b \nabla_c k_a + R_{cba}^\ d k_d) = \nabla_b (k^c \nabla_c k_a) - (\nabla_b k^c) (\nabla_c k_a) + R_{cba}^\ d k^d = -B^e_{\ bc} \omega_c + R_{cba}^\ d k^d$ (6)

where we used the Leibniz rule, the geodesic equation and the relation $(\nabla_b \nabla_a - \nabla_a \nabla_b) \omega_a = R_{abc}^\ d \omega_d$, valid for any smooth dual vector field $\omega_\nu$, which introduces the Riemann curvature tensor $R_{abc}^\ d$.

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$\theta = B^a_b = (\kappa^{-1})^a_{\ bc} k^c \kappa^a = k^b \nabla_b \log |\det \kappa^a|$

diverges when $\kappa^a$ becomes degenerate

From the geodesic deviation equation (6) we obtain the Raychaudhuri equation as its trace:

$\dot{\theta} = k^c \nabla_c \theta = 8 \epsilon^{abcd} k^c \nabla_c B_{ab} = -\frac{1}{2} \theta^2 - \sigma_{ab} \sigma^{ab} + \omega_{ab} \omega^{ab} - R_{ab} k^a k^b$.

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$3$ We have used $(\det \kappa^a)^{-1} \nabla_b \det \kappa^a = (\chi^{-1})^a_{\ bc} \nabla_c \kappa^a$ which follows easily from $\det \kappa^a = \frac{1}{4} \epsilon_{abcd} k^c k^d \chi k^a k^b k^c k^d$.

$4$ For a geodesic congruence one can see, using the Frobenius theorem, that this is realized whenever the congruence is orthogonal to a hypersurface.
FIGURE 4. Causal diagram in spherical coordinates showing the ingoing null geodesic family of a 2-sphere centered at the origin of spherical coordinates. The family has a focal point at the origin (left vertical line). Any point beyond the focal point can be reached by a time-like curve from the initial 2-sphere.

then $\theta$ always decreases along geodesics in the family. This is the focusing effect of gravity and plays a major role in deriving singularity theorems.

Quantitatively, we have $\dot{\theta} \leq -\frac{1}{2} \dot{\theta}^2$ such that after integration $\theta^{-1} \geq \theta_0^{-1} + \frac{1}{2}(t - t_0)$ starting from initial values $\theta_0$ at $t = t_0$. This is the place where initial values for geodesic families enter. For negative $\theta_0$, $\theta$ must diverge after finite time no larger than $t - t_0 = 2/|\theta_0|$. Geodesics must intersect before that time and form a caustic (focal point).

2.2.2. From caustics to singularities

Caustics are singularities where a geodesic family ceases to define a smooth submanifold of space-time. But they are not physical singularities since space-time itself is usually well-defined at points where light rays intersect. To relate the occurrence of caustics to space-time singularities we need one more ingredient beyond the initial conditions and positive energy assumptions together with Einstein’s equation already used.

The required basic statement from differential geometry is the well-known property of geodesics as extremizing arc-length. Space-like geodesics extremize arc-length $\ell_e = \int_e \sqrt{g_{ab} \dot{e}^a \dot{e}^b} dt$ among curves between two given points and minimize it unless there is a focal point between the two points. Similarly, time-like geodesics extremize proper time $\tau_e = \int_e \sqrt{-g_{ab} \dot{e}^a \dot{e}^b} dt$ between two points and maximize it unless there is a focal point between the two points. For a null geodesic such an extremization condition is not possible since the norm of a null vector vanishes and thus any null curve has zero length. But there is an analog to the statement that minimization of arc-length by space-like geodesics or maximization of proper time by time-like ones ceases beyond focal points: Any point on a null geodesic beyond a focal point can be reached by a time-like curve. In a causal diagram in spherical coordinates, this is depicted in Fig. 4.

According to the Raychaudhuri equation, together with the usual assumptions of positive energy, every null normal geodesic family starting from a trapped surface must develop a focal point since the initial expansions are negative by definition of a trapped surface. This is always realized for ingoing geodesics, but can it be possible for outgoing ones? There is no difficulty if space is compact, as shown in the left part of Fig. 5 since there will be another coordinate center or a periodic identification encountered by the outgoing family. In fact, for a compact spatial manifold one cannot clearly distinguish between ingoing and outgoing null normals of a 2-dimensional space-like submanifold. But for non-compact spatial topology the outgoing null geodesics continue to go on forever and can never be caught up with by a time-like geodesic.

There is thus a contradiction between the Raychaudhuri equation, in the context of positive curvature and given the existence of a trapped surface, and space-time topology for non-compact space. At this stage, finally, topological conditions are needed and we are able to translate caustics of geodesic families into space-time singularities. The contradiction can only be avoided by concluding that incomplete geodesics exists. The outgoing geodesic family does not develop a focal point, despite of the Raychaudhuri equation, because it can simply not be extended arbitrarily. When we formulated the contradiction there was the hidden assumption that the null geodesics in the family can be extended arbitrarily, i.e. we assumed them to be complete. The only way to avoid the contradiction is to conclude that incomplete null geodesics must exist: space-time is singular in the sense of geodesic incompleteness (see the right part of Fig. 5).
FIGURE 5. Causal diagrams of a spatially compact manifold with two focal points of null geodesic families (left) and of the outgoing null geodesic family encountering a space-time singularity in the spatially non-compact case (right).

2.2.3. Scheme of singularity theorems

The proof sketched above illustrates the general assumptions and conclusions used in singularity theorems:

1. **Initial conditions** ensure the existence of geodesic families with negative expansion. Typical cases are trapped surfaces, implying black hole singularities, or spatial slices whose expansion or contraction is bounded away from zero everywhere, giving rise to cosmological singularities.

2. Using **positive energy conditions** together with Einstein’s equation in the Raychaudhuri equation implies focusing. With the initial conditions specified, caustics develop in finite time.

3. A caustic in general is only a “singularity” of the geodesic family, not of space-time. A singularity theorem finally results together with **topological assumptions** rendering a caustic into an obstruction to geodesic completeness.

An important consequence is that dynamics of the gravitational field is not used very specifically, but only to translate positive energy conditions into focusing.

2.2.4. Example: Schwarzschild geometry

In general, it can be difficult to identify all trapped surfaces in a given space-time, but spherical trapped surfaces in a spherically symmetric spacetime are simple to detect. (See, e.g., [8, 9] for non-spherical trapped surfaces.) We use this here as an example to illustrate the relation between the regions where trapped surfaces occur and space-time singularities. With a line element

\[ ds^2 = -N(r,t)^2 dr^2 + R(r,t)^2 d^2 + r^2 d\Omega^2 \]

formulated in the “area radius” \( r \), we consider submanifolds defined by \( r = r_0 \) being constant. This is usually a time-like submanifold as illustrated in the left part of Fig. 6. While the ingoing null geodesic family moves toward smaller \( r < r_0 \) and is contracting, the outgoing null normal geodesic family moves to larger \( r > r_0 \) and is expanding. Such a 2-sphere obtained as the cross section of a time-like constant-\( r \) surface is thus untrapped. When the submanifold \( r = r_0 \) is space-like, by contrast, both the ingoing and outgoing null normal geodesic families move to smaller \( r \) (or larger depending on whether the surfaces are future or past trapped); see the right part of Fig. 6. Any cross section of a space-like constant-\( r \) surface is thus trapped.

Thus, whenever \( n_a (dr)_a \) is time-like, \( g^{ab} n_a n_b = R^{-2} < 0 \), we have trapped surfaces. (If we use a line element with non-zero shift \( N_t = g_{rr} N^r \), the inequality reads \( g^{rr} = (R^2 N^2 - N^2_r) / N^2 R^4 < 0 \).) For the Schwarzschild solution \( R^{-2} = 1 - 2M / r \), and any sphere with \( r_0 < 2M \) is trapped. To the future of this region there must thus be a singularity, as it is drawn in the usual conformal diagram Fig. 7.

2.3. General situation and Alternatives

Singularity theorems demonstrate the stability under non-symmetric perturbations of singularities explicitly seen in symmetric solutions, such as the Schwarzschild or homogeneous cosmological solutions. Historically, this played an important role in accepting the importance of singularities for solutions of general relativity. But as in any mathematical theorem, assumptions are certainly necessary. The most general theorems, those with the weakest assumptions, only
show that one incomplete geodesic exists. Moreover, the general structure (such as curvature divergence) is not illuminated at all. The significance of singularity theorems can thus be questioned, and indeed non-singular (though maybe not fully realistic) solutions exist even if positive energy conditions are assumed \[10, 11\].

Nevertheless, no general conditions for non-singular solutions are known, and thus singularities cannot be ignored in general relativity. Generic solutions have boundaries which cannot be penetrated by geodesic observers provided that positive energy conditions hold. General relativity is thus incomplete as it does not show what happens at and beyond boundaries of its solutions. Extensions of the theory are necessary. The key to solving the singularity problem is not to find non-singular solutions but to provide sufficiently general conditions under which non-singular behavior would be guaranteed. This is not available in classical gravity even if no energy conditions are imposed at all.

Rather than using geodesic completeness as a criterion for non-singular behavior, one can use alternative conditions for non-singular space-times. One that is more physically motivated is generalized hyperbolicity \[12\] which states that all space-times allowing a well-posed initial value problem for standard matter fields are to be considered non-singular. This uses physical, potentially fundamental fields rather than test particles. It is more general since (conical space-time) solutions are known which are geodesically incomplete but satisfy generalized hyperbolicity \[13, 14\]. However, no general results are available at present while the usual cosmological and black hole singularities certainly present counter-examples.

Instead of changing criteria for singularities, modifying gravity might lead to better situations: examples include alternative degrees of freedom such as test strings rather than particles in string theory or properties of quantized space-time in quantum gravity as they will be discussed in the next section.

### 3. BEYOND GENERAL RELATIVITY

Singularity theorems demonstrate geodesic incompleteness under quite general assumptions, based mainly on differential geometry (the geodesic deviation and Raychaudhuri equations) in combination with positive curvature. This implies focusing of geodesic families which, together with topological conditions, result in space-time singularities. But special non-singular solutions do exist classically, so the question is not if one can avoid the conclusions by evading assumptions. What is missing is a general mechanism by which one can conclude non-singular behavior in a sufficiently general class of physical situations.

Violating energy conditions is an obvious candidate to evade the usual singularity theorems, but even this does not work generally enough for the types of matter we seem to need for fundamental physics. Singularity theorems have been proven, with different assumptions, for instance in the context of inflaton fields which violate positive
energy conditions [13]. Moreover, dropping positive energy assumptions does not necessarily improve the situation but usually makes it worse as the development of sudden future singularities in so-called phantom matter field models shows [16].

Other than that, only modifications of gravity itself rather than matter can help. But also this will be subtle because not much of general relativistic dynamics is being used in singularity theorems.

3.1. Facets of the singularity problem

The singularity problem is a complicated issue to be addressed in a more general theory of gravity, extending general relativity in a well-defined form. For any explicit discussion, the main difficulties are:

1. No general classification of singularities is available and many different types exist.
2. Singularities are not always accompanied by unbounded curvature as in the best known examples. It is thus not sufficient to address only unbounded curvature because this is not even shown in singularity theorems.
3. In fact, not all singularities should be resolved [17]. Some are useful to rule out negative mass, e.g. of the Schwarzschild solution. Such singularities are typically time-like rather than space-like which is an important additional property not covered in singularity theorems.

In isotropic models, one can often construct bounce pictures where the volume of any solution is bounded away from zero. This can be achieved by appropriate modifications of the dynamics which avoid unbounded curvature. But such models do not serve as a general mechanism.

Curvature singularities, although not necessarily implied by the singularity theorems, are the best known types realized in cosmology and black hole physics. They can often be dealt with in special ways which more or less directly ensure bounded curvature. In particular, large curvature implies high energy regimes of field theories defined on a singular gravitational background. As usually, field theories are expected to receive strong quantum corrections in high energy regimes which, when even the gravitational field is at “high energies” in the sense of strong curvature, may also modify gravitational dynamics itself. General relativity would then only be obtained as an effective description, or the small curvature limit of a suitable extension valid also at high curvature.

In quantum field theory and condensed matter physics, effective descriptions on small energy scales or large length scales can be defined by integrating out “massive” or short wave length degrees of freedom which will become important at high energies. At low energies those modes can safely be ignored, but they will become relevant when typical energies reach their mass or when the curvature radius approaches their length scale. Ignoring the additional degrees of freedom in such a situation implies deviations, or possibly a failure of the low energy description in the form of singularities. It is then only the effective description which fails and appears to be singular while the more fundamental theory can (and should) be non-singular.

This is an interesting and partially successful picture for which many examples are available. Most of these examples are motivated by special known solutions (mainly Friedmann–Robertson–Walker ones) and devised with cosmological bounces in mind. So far, they are not general enough to extend to more complicated, especially inhomogeneous, solutions. Moreover, they do not address the true problem of gravitational singularities: not all singularities have large curvature, and diverging curvature is not the basic mechanism behind singularity theorems. By addressing exclusively unbounded curvature one appears to be treating a symptom rather than the cause.

3.2. Example: string theory

String theory [18] provides an example for a theory whose dynamics reduces to that of general relativity for small curvature and low energies but differs at large energies. In particular, string theory can be quantized perturbatively which is not the case for general relativity without high energy corrections. Conceptual features are, however, quite different in string theory. For instance, while solutions of general relativity are not just a metric perturbation but rather the space-time manifold itself, as discussed before, string theory in its present version formulates gravitational excitations on a given metric background. This certainly has implications for how generally the singularity issue can be addressed, keeping in mind that singularities in general relativity are understood as boundaries of space-time arising through the dynamical laws that govern its own structure. If a background manifold is put in from the outset, a discussion and resolution of singularities at a general level becomes impossible. String theory does, however, provide
valuable insights into how special singularities can be resolved by new degrees of freedom. This occurs mainly through a different viewpoint on test objects replacing geodesics, and through candidates for massive degrees of freedom not contained in general relativity. Many examples are discussed, e.g., in the recent review [19] to which we refer for details and more complete references.

In string theory, one uses 1-dimensional strings or higher dimensional branes rather than pointlike particles as basic objects. World-volumes of test strings or branes then replace geodesics followed by point particles as the submanifolds whose incompleteness would signal a singularity in the spirit of general relativity’s singularity theorems. This has been shown to change completeness results and lead, in this sense, to more regular behavior especially for conical or orbifold singularities (which are not space-like). It also provides examples for new degrees of freedom which, when taken into account rather than being integrated out, are necessary for regular behavior [20].

This, however, has been difficult to extend to dynamical space-times such as those displaying curvature singularities. General arguments why such space-times provide a qualitatively different challenge have been presented in [21], and several so far unsuccessful alternative attempts can be found in [22, 23]. The main difficulty is that string perturbation theory generally breaks down in such space-times. (Perturbation theory might be useful for the singularity issue in the context of tachyon condensation [24], but has so far been used only for null singularities where curvature does not diverge.)

A second source of additional degrees of freedom which could become light close to a classical singularity and help to resolve it are string winding modes around topologically non-trivial components of space-time (or brane separation parameters): their mass $m \propto R^{-1}$ is proportional to the inverse radius (measured in the background metric the strings are propagating in) of the compact direction they are winding around. This is highly massive, and thus negligible in low energy effective theory, if extra dimensions are small, but can become relevant in high curvature regimes. It has been shown that winding modes can easily lead to bounces [25], but typically only of some directions. With small extra dimensions one is necessarily dealing with anisotropic geometries such that a bounce in one direction does not imply a spatial volume bounded away from zero. Usually, only the compact dimension bounces. Moreover, by design special topologies or configurations are required for winding modes to exist which spoils prospects for a general mechanism as gravitational singularities also occur in simply connected space-times.

These constructions referred to strings propagating in non-evolving backgrounds. It is much more difficult to find analogous mechanisms in dynamical space-times as they arise in cosmology or in the interior of black holes close to their singularities. In such a context, not only technical difficulties arise but also applications of low-energy effective actions, which are mainly being used to study the effect of massive degrees of freedom, are not always general enough [26]. While low energy effective actions are well-suited to study the propagation and scattering of fields which are not highly excited out of their vacua, dynamical space-times in quantum gravity have to include a gravitational state far away from its vacuum. Then, more general effective equations are necessary which, requiring good knowledge of the quantum gravity state, are more complicated to derive.

The main difficulty is that in all examples one is still using test objects in a background space-time, such as new fields provided by positions of branes. This does not include the dynamics of space-time itself. Moreover, strong back-reaction effects occur [27, 23] showing that gravitational dynamics is very relevant and that a pure background treatment is insufficient. The most detailed scenario in this context has been formulated for the Schwarzschild-AdS singularity, rather than a dynamical cosmological one. From an analysis of correlation functions of the conformal boundary field theory one can conclude that bulk properties such as horizons and singularities only emerge in the classical limit but are not present in quantum gravity [28].

Tight arguments have been put forward which indicate that bounces found in homogeneous models are unlikely to extend to inhomogeneous situations [29]. Although they have been discussed there mainly in the context of the AdS/CFT correspondence, some of the arguments are general enough to caution against direct generalizations of homogeneous results in any context, not just in string theory. Specifically, an upside-down potential for field modes is argued to arise in a boundary field theory description of the cosmological situation. Field modes in this potential will reach infinity in a finite amount of time, corresponding to the classical singularity. Since all modes are independent, they behave differently even if they started out in a highly correlated manner from an isotropic initial configuration. Quantum gravity, by way of a self-adjoint extension of the field Hamiltonian which leads to reflecting boundary conditions at infinite values of the fields, could make the behavior non-singular. But if this happens, the field modes are unlikely to return to an highly correlated state as the initial one. Thus, while evolution of the quantum theory continues, it does not easily lead to a classical bounce back to a classical geometry. The main property of inhomogeneities used in this argument is the large number of fundamental degrees of freedom, which all need to be re-excited collectively in a special way for a smooth bouncing geometry to result. Independently of the specific quantization of inhomogeneities, this is much easier to achieve in homogeneous models with a small number of degrees of freedom.
than in inhomogeneous ones.

### 3.3. Geometry

Singularity theorems are mainly statements about differential geometry as they refer to properties of geodesics on a curved manifold. Einstein’s equation is used only at one place, relating positive energy to positive curvature, which then implies focusing effects in the Raychaudhuri equation. Focusing through positive energy is used in the most common theorems, but is not the only reason since singularities easily arise with violated energy conditions.

For a general solution of the singularity problem one should thus focus on geometry, not just on dynamics. Although both are intertwined in general relativity, geometry determines which type of dynamics is possible such that it can be viewed as more basic. Rather than modifying gravitational dynamics in a given geometrical setting, using a different geometry could be much more successful to avoid the far-reaching conclusions of singularity theorems.

An alternative geometry is automatically provided by background independent quantizations, such as canonical quantizations. Such theories are not based on objects in a background space-time but they quantize full metric components as the non-perturbative dynamical objects. For instance, most versions employ wave functions supported, e.g., on the space of spatial metrics \( q_{ab} \) which is the configuration space of canonical general relativity. Geometrical objects then become operators acting on these wave functions with properties generally very different from classical smooth geometry. A new quantum geometry underlying gravity then arises with an entirely new setting for the singularity issue. Despite of the difference to classical geometry, for any consistent quantum theory of gravity smooth space-times have to be approached as a classical limit far away from singularities. But large deviations from classical behavior can occur around classical singularities, possibly resulting in regular equations. Quantum geometry then, if this picture is successful, provides links between classical parts of space-time which would otherwise be interrupted by singularities.

Canonical techniques treat space and time differently because time derivatives of fields are replaced by momenta but their spatial derivatives are retained. This is also true in relativistic theories where manifestly covariant theories are rewritten canonically in a form referring separately to space and time. Although this hides the covariance of field equations, constraints ensure that solutions still respect the equivalence principle.

In general relativity, a canonical formulation is defined by introducing a foliation of space-time into a family of spatial slices in terms of a time function \( t \) such that the slices are \( \Sigma_t : t = \text{const.} \). Moreover one chooses a time evolution vector field \( t^a \) such that \( t^a \nabla_a t = 1 \) which determines how points on different spatial slices are identified (along integral curves of \( t^a \)) to result in spatial fields “evolving” in coordinate time \( t \). In addition to the time evolution vector field there is the geometrically defined unit normal vector field \( n^a \) to the spatial slices in space-time. This allows one to decompose the time evolution vector field \( t^a = N n^a + \Sigma^a \), as illustrated in Fig. 8 into a normal part, whose length is given by the lapse function \( N \), and a tangential part given by the spatial shift vector \( \Sigma^a \). One can then split off the time components from the inverse metric \( g^{ab} \) by defining the inverse spatial metric \( q^{ab} = g^{ab} + n^a n^b \) such that \( q^{ab} n_b = 0 \). Thus, the spatial metric indeed has only components tangential to spatial slices. Solving the relation for

\[
g^{ab} = q^{ab} - n^a n^b = q^{ab} - \frac{1}{N^2} (t^a - N^a)(t^b - N^b)
\]

and inverting it results in the space-time metric (1) in the canonical form already used before. As is clear from the construction, lapse function and shift vector arise through the space-time foliation and define coordinate time evolution through the way different spatial slices are identified. They are thus related to the space-time gauge but are not dynamical fields. This confirms the realization that they are not subject to evolution equations as their time derivatives do not occur in Einstein’s equation.

Evolution equations do result for the spatial metric \( q_{ab}(t) \), interpreted as a time dependent field through its values on different \( \Sigma_t \). In a canonical formulation we have first order equations (2) and (3) for \( q_{ab} \) and its momentum, related to extrinsic curvature \( K_{ab} = \frac{1}{2\kappa} (\mathcal{L}_t q_{ab} - 2D_a N_b) \) of \( \Sigma_t \) (with \( \mathcal{L}_t \) denoting the Lie derivative along \( t^a \)). These phase space coordinates given by spatial metric components \( q_{ab} \) and their momenta are subject to constraint equations (4) implementing their dynamics, as we will discuss in more detail in the next section. For now, it suffices to know that, when quantized, wave functions on the space of metrics (if a metric representation is chosen) arise which are subject
to differential or difference \(\text{diff}^5\) equations depending on the quantization scheme.

There are then no test objects in a background space-time, but wave functions or gravitational observables are the fundamental dynamical entities. Differential geometry becomes applicable only in a classical approximation to describe space-time, and only in classical regions would geodesics be defined at all. Geodesic incompleteness is thus inapplicable as a criterion for singularities in quantum gravity. This suggests a natural answer to why incompleteness occurs so generally in general relativity: geodesics themselves are only valid as long as a differentiable classical geometry can be assumed. (In fact, there are cases of geodesic incompleteness where simply the metric ceases to be differentiable. These are typically the examples where generalized hyperbolicity as a criterion leads to non-singular space-times although they would be geodesically incomplete.) When quantum geometry becomes relevant, geodesics stop and have to be replaced by something more appropriate. Only classical geometry would end, but not quantum gravity with its own version of quantum geometry. Such a scenario looks promising but it has to be developed and verified in detail, requiring explicit candidates for background independent quantum gravity such as a canonical quantization. The question then remains: How do we address or even define singularities in such a context?

3.4. Quantum hyperbolicity

Classical singularities refer to properties of spacetime as a metric manifold. Abstractly, they are thus identified through properties of the metric tensor on certain submanifolds, although an explicit classification in general terms is lacking. In a canonical quantization, classical singularities must then correspond to properties of states, or of suitable observables in a Heisenberg picture. The usual example is how a wave function in the metric representation is supported on certain submanifolds of the space of spatial metrics which classically would imply a singularity. Before we can even use quantum dynamics we must be able to provide an unambiguous one-to-one correspondence between classical singularities and metric tensors. This could to some extent be done in terms of curvature invariants, but must be more general since not any singularity refers to curvature. Such a classification is not available in full generality and is thus the major difficulty in any general discussion of the singularity problem in quantum gravity, irrespective of the specific quantization approach followed.

Although a general classification is not available, a new criterion for gravitational singularities becomes possible: If a state can uniquely be extended across or around all submanifolds of classically singular configurations they do not pose obstructions to quantum evolution in any sense. If, however, a state such as a wave function on the space of metrics cannot be extended uniquely across a classically singular submanifold, there would still be a boundary to quantum evolution and quantum space-time would remain incomplete. This viewpoint is the natural extension of generalized hyperbolicity from matter fields on space-time to the fundamental object of quantum space-time itself. We therefore call it the principle of quantum hyperbolicity.

A verification in concrete ways requires quantum geometry for the location of potential singularities and quantum dynamics to see if states can uniquely be extended across such places. The set-up in this form is general without specific reference to unbounded curvature. It can potentially deal with the general types of singularities implied by the theorems.

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5 Whenever we write “\(\text{diff}^5\)” we mean that differential or difference equations can occur depending on the context (the quantization scheme used) but the statement does not depend on the type of equation.
States, as solutions to the dynamical equations of quantum gravity, thus have to be extended uniquely across classical singularities. As a general principle, it entails several sub-issues necessary for its verification:

- First, phase space locations of classical singularities in terms of metric or curvature components have to be unambiguously identified.
- The structure of submanifolds in phase space corresponding to classical singularities according to the first point then determines how the classical space of metrics is separated into several disconnected components. In some sense to be specified, any state has to be extended uniquely between any two such regions. This gives meaning to an extension of states across classical singularities.
- Before this extension can be shown to exist uniquely, representations of states or relational observables must be chosen. The formulation of an extension is necessarily representation dependent because, for instance, no background coordinates are available in which classical metrics $g_{ab}(t)$ would approach a singularity. Any extension is thus provided in phase space variables (internal time) which are monotonic around a classical singularity. This selects representations in which one observes an extension of a wave function from one part of its support to another, rather than a superposition of different branches.
- Finally, the dynamical equations of quantum gravity will be used to verify that all states can be extended in the way envisioned in earlier steps. For a general answer to the singularity issue it is important to prove this extension for all allowed states rather than for restricted classes such as those given by one specific initial condition.

For a specific proposal of how quantum hyperbolicity could be realized, one can use the usual Wheeler–DeWitt type wave functions on the space of metrics $[30,31]$. Then, metric variables would be used to provide extensions across a classical singularity. The first point above, classifying classical singularities through the metric behavior, cannot be performed currently in full generality, but is often easily available in symmetric models. One thus studies mini- or midisuperspaces of metrics respecting a certain symmetry and possible extensions of wave functions within this class of metrics. Also quantum dynamics can often be obtained explicitly in such models such that the program can be carried through. Also here, one has to be careful with interpreting results in any given model because the structure of classical singularities as well as quantum dynamics are truncated by restricting oneself to one class of metrics. But the investigation of several different models, covering different types of classical singularities, provides valuable information as to whether or not a general mechanism providing quantum hyperbolicity can exist. It also shows how details of the specific quantum theory of gravity used in the process matter which allows conclusions about general constructions.

If realized, quantum hyperbolicity provides a quantum version of generalized hyperbolicity and thus deals with the well-posedness of evolution problems. If quantum equations of wave functions are well-posed, there are no boundaries for quantum evolution even where one would classically expect a singularity. Given that issues of hyperbolicity are very difficult in general relativity and generalized hyperbolicity at the classical level has not been studied much one could question the feasibility of quantum hyperbolicity as a verifiable criterion in quantum gravity. After all, quantum dynamics is expected to be much more complicated than classical dynamics from a mathematical point of view. In fact, quantum dynamics in background independent approaches has not even been fully formulated yet. Nevertheless, quantum theory allows an important simplification of testing well-posedness: If one uses a Schrödinger picture of states, dynamical equations are linear. This removes one of the major difficulties present in classical general
relativity. The complicated issue is, of course, to extract observable information out of the states where the non-linearity of gravity enters. Moreover, solutions even to linear quantum equations can be difficult to find explicitly in inhomogeneous models with many independent degrees of freedom. But for hyperbolicity we only need to study the well-posedness of initial or boundary value problems without the need of having explicit solutions available. This is much more feasible for linear compared to non-linear equations. Then, given that states can be uniquely extended across classical singularities once quantum hyperbolicity has been verified, one is assured that observable information extracted from such extended states also reaches from one disconnected part of classical superspace to others. This is a hopeful sign that general statements about the singularity issue can be made in quantum gravity without having to face all the difficult issues, just as singularity theorems were derived in classical gravity without much knowledge about the general solution space.

### 3.4.1. Examples: isotropic, homogeneous space-times and the BKL conjecture

Nevertheless, simple examples demonstrate that there are many non-trivial issues in verifying quantum hyperbolicity. The general idea is best illustrated in isotropic models with a single metric component given by the scale factor $a > 0$, subject to the Friedmann equation $(\dot{a}/a)^2 = \frac{8\pi G}{3}\rho(a, \phi)$. Classical singularities for the usual matter contributions, such as a scalar field, are reached at $a = 0$. This gives a simple and general identification of classical singularities for isotropic geometries. Since $a$ is positive, the classically singular submanifold is a boundary rather than an interior submanifold. Wheeler–DeWitt wave functions in the metric representation take the form $\psi(a, \phi)$ with a scalar field $\phi$ assumed as the matter content.

This provides the simplest situation, but is very special. Even keeping homogeneity, the situation changes considerably if anisotropy is allowed such as in the Bianchi I model. There are then three independent metric components $a_I > 0$, $I = 1, 2, 3$, determining a metric $\text{d}s^2 = -\text{d}t^2 + \sum_I a_I^2 (\text{d}x^I)^2$. Instead of the Friedmann equation, we have the constraint $\dot{a}_1 \dot{a}_2 + \dot{a}_1 \dot{a}_3 + \dot{a}_2 \dot{a}_3 = 0$ which is solved by the Kasner solutions $a_I \propto t^\alpha_I$ where $\alpha_I$ are real numbers such that $\sum_I \alpha_I = 1 = \sum_I \alpha^2_I$. These two equations have only solutions (except for the non-dynamical one corresponding to Minkowski space) satisfying $-1 < \alpha_I \leq 1$. One of them must then be negative while the other two are positive. The total volume is proportional to $a_1 a_2 a_3 \sim t$ which vanishes at $t = 0$, corresponding to the classical singularity. Again, we have a simple characterization, but now the behavior of the metric components is very different: one metric component diverges at the singularity. The singular submanifold is thus not only a boundary but located at infinity. This makes investigating the well-posedness of initial value problems of wave function $\psi(a_1, a_2, a_3)$ in a neighborhood of the classical singularity more complicated.

In any case, it demonstrates that conclusions drawn from isotropic models cannot easily be generalized because the structure of classical singularities themselves changes. On the other hand, there are indications related to the BKL conjecture [32] that anisotropic models are quite generic and provide crucial information even for inhomogeneous situations. In this context one is looking for generic asymptotic solutions close to a space-like curvature singularity at $\tau = 0$, which are argued to be of the form

$$\text{d}s^2 = -\text{d}t^2 + t^{2\alpha_1} (\omega_1)^2 + t^{2\alpha_2} (\omega_2)^2 + t^{2\alpha_3} (\omega_3)^2.$$ 

Thus, a homogeneous Bianchi model, whose invariant 1-forms $\omega^*_a$ are used in the spatial part of the metric, is generalized by allowing position dependent Kasner exponents $\alpha_I(x)$. For a Bianchi I model, for instance, one would simply have $\omega^*_I = \text{d}x^I$ in terms of Cartesian coordinates $x^I$. More generally, the 1-forms $\omega^*_a$ are left invariant 1-forms on a 3-dimensional Lie group and thus satisfy the Maurer–Cartan relations $\text{d}\omega^*_I = -\frac{1}{2} C^*_IJK \omega^*_J \wedge \omega^K$ with the structure constants $C^*_IJK$ of the Lie algebra.

Since inhomogeneities in this class of space-times are modeled by space dependent exponents $\alpha_I(x)$, there are gradient terms containing the spatial derivatives $\partial_a \alpha_I$ added to the homogeneous equations of motion. This can be derived from the Christoffel connection which, in addition to the terms occurring in a homogeneous model with constant $\alpha_I$, receives contributions

$$\delta^{(3)} \Gamma^{c}_{ab} = \frac{1}{2} q^{cd} (\partial_a \delta q_{bd} + \partial_b \delta q_{ad} - \partial_d \delta q_{ab})$$

where $\delta q_{ab} \text{d}x^a \text{d}x^b = \sum_q (t^{2\alpha_1(I)} - t^{2\alpha_1}) (\omega^I)^2$ is the difference spatial metric after introducing inhomogeneity. This term can easily be computed:

$$\delta^{(3)} \Gamma^{c}_{ab} = \log \tau (\delta^*_c \delta_a \alpha_{(b)} + \delta^*_a \delta_b \alpha_{(c)} - \delta^{cd} \delta_{ab} \delta_c \alpha_{(d)})$$

(8)
which diverges logarithmically at $\tau = 0$. Thus, 3-curvature terms of $(3)R_{abc}^d$ resulting from this contribution, diverge as $(\log \tau)^2$, and the 3-Ricci scalar as $e^{2\alpha_2}(\log \tau)^2$.

This is to be compared to contributions of the homogeneous curvature scalar to see if inhomogeneities play a role for curvature and equations of motion. For a general Bianchi class A model with structure constants parameterized in the form $\epsilon_{ijk}^\alpha = \epsilon_{njk} n^{(i)}(\alpha)^{n} = \alpha^{n}$ we have the 3-Ricci scalar

$$\tag{9}
(3)R_{\text{hom}} = -\frac{1}{2} \left( n^1 q_1 q_3 + n^2 q_2 q_3 + n^3 q_1 q_3 - 2 n^1 n^2 q_2 - 2 n^1 n^3 q_1 - 2 n^2 n^3 q_1 \right)
$$

for a diagonal metric of the form $q_{IJ} = q_{IJ}^I$ in the $\alpha^I$-basis. Assuming, without loss of generality, that $\alpha_1 < 0$ is the negative one of the Kasner exponents, the strongest divergence of $(3)R_{\text{hom}}$ is given by $q_{1}^I q_{2}^J q_{3}^1 \sim e^{2\alpha_1 - 2\alpha_2 - 2\alpha_3}$. Since $2\alpha_1 - 2\alpha_2 - 2\alpha_3 < 2\alpha_I$ for all $I$ if $\alpha_I$ is the negative exponent, the homogeneous contribution is more divergent than the gradient contributions resulting from $q_{1}^{I} q_{2}^{J} q_{3}^{I}$. This gives rise to the conjecture that spatial derivatives are subdominant asymptotically close to the singularity and that a general solution behaves locally as a homogeneous model of the Bianchi IX form ($n^1 = n^2 = n^3 = 1$) where all diverging terms in $(3)R_{\text{hom}}$ are present.

However, the BKL conjecture, although by now strongly supported [34, 35], has not been proven, and it is even less secure that it will extend to a quantum version. Diverging curvature is relevant in the argument, and it thus refers explicitly to curvature singularities. Classical equations of motion have been used which themselves may change in such strong quantum regimes. Moreover, one must get close to the classical singularity in order to have subdominant spatial gradients. Bounce models, as they are often discussed, avoid this high curvature regime and cannot appeal to the BKL conjecture to justify a possible extension to inhomogeneous situations. Thus, inhomogeneous models as close to the full situation as possible must still be considered in detail.

### 3.4.2. Boundaries

As seen in the examples, when metric variables are used for a characterization, singularities usually appear at boundaries of superspace since $\det g_{ab} > 0$ by definition and singularities often have degenerate metric or triad components. This makes it difficult to extend states across such submanifolds; one could at most ask that the state at the classical singularity be well-defined and that, in a certain sense, the boundary does not pose an obstruction to physical evolution. This suggests, as it is often used, to impose boundary conditions on wave functions right at a classical singularity, with different motivations for specific proposals [36, 37, 38]. If these are conditions which imply, for instance, wave packets being reflected off the boundary, one can argue that evolution is not interrupted. Such an interpretation is, however, not easy to justify in general. It is dependent on choices of the precise form of boundary conditions and difficult to make generic beyond isotropic models. Even if the wave function is not supported at a classical singularity, it does not mean that all extracted physical information is regular. To test this one would have to construct observables and the physical inner product in order to compute expectation values. If all these quantities remain regular, one can conclude that the classical singularity has been resolved. But if only wave functions have been shown, or restricted by boundary conditions, to remain regular one is not in a position to decide about singularity resolution. For instance, while a wave function constrained to vanish at $a = 0$ of an isotropic model taken together with the usual probability interpretation (which is itself subject to difficult interpretational issue in quantum gravity) implies directly that any physical quantity is supported only away from zero, it does not lead to general lower bounds for $a$. While in any given state the expectation value of $\hat{a}$ in the usual inner product would have a positive lower bound, one can always choose a state where the expectation value comes arbitrarily close to zero. The boundedness of $a$ is then only put in through selecting the particular boundary condition, but cannot be regarded as a consequence of quantum gravity. Moreover, the physical inner product in which one computes the expectation value might itself contribute a function of $a$ diverging at $a = 0$. While one can sometimes compute the physical inner product in specific models, which does not only involve assuming symmetries but also selecting the matter content, there is no general information on its behavior. Any interpretation of properties of wave functions which relies on the physical inner product is thus highly difficult to turn into a general argument to address the singularity issue.

Probably the most advanced discussion in this context can be found in the application [39, 40] to gravitational collapse. It is shown there that a canonical quantization of the explicitly determined reduced and deparameterized phase space (i.e. an internal time has been introduced to describe physical evolution), which solves all the constraints, is non-singular in the sense that an initial wave packet not supported at the classical singularity always vanishes at the classical singularity. This provides a full analysis making use of Dirac observables and a physical inner product.
It is by far the strongest result in this context. Nevertheless, the question of whether it can be extended to a general mechanism remains open. First, the direct use of Dirac observables, although necessary to discuss singularity removal possibly implied by boundary conditions of wave functions, makes it difficult to see what happens in other situations where Dirac observables are rarely known explicitly. The very fact that Dirac observables can be computed explicitly in this model may imply that it is quite special, including its dynamics. But more importantly, the mechanism in the collapse model depends on assumptions on a semiclassical initial state: One must assume that the initial state is not supported at all at the classical singularity but only at a peak value far away. Then, unitary evolution preserves the boundary condition which guarantees that the wave function will never be supported at the classical singularity. While this looks innocent, it makes singularity removal in this scheme unstable: If there is only a tiny contribution to the wave function not vanishing at the classical singularity, it would not change much of the initial semiclassical behavior. But this already spoils the preservation of the boundary condition and in general a wave packet approaching the classical singularity will not stay away from it completely. The mechanism, like others based on boundary conditions, is thus sensitive to precise details of physics at the Planck scale which have to be dealt with by extra assumptions.

Classical singularities located at boundaries of the space of metrics thus do not offer an obvious general and verifiable way for regular behavior. Quantum hyperbolicity does not require explicit observables but can be formulated directly for general states solving the dynamical constraints. Nevertheless, a location of classical singularities at boundaries seems to prevent the applicability of quantum hyperbolicity in any realistic sense because the choice of boundary data matters crucially. But one should note that the characterization of classical singularities as kinematical boundaries in this way depends on the variables used. The main reason for the location at boundaries was the restriction $\text{det} q_{ab} > 0$ which obviously has to be imposed on the spatial metric. But geometry can just as well be described in triad variables, which is even necessary if fermionic fields are present. If a co-triad $e^i_a$ is being used, defined as three co-vector fields $e^i_a$, $i = 1, 2, 3$ such that $\Sigma e^i_a e^i_b = q_{ab}$, the sign of $\text{det} e^i_a$ is relevant since it determines the orientation of space while $\text{det} q_{ab}$ will still be non-negative. A surface $\text{det} e^i_a = 0$ is then interior, not a boundary.

A quick look at the models studied before reveals that this sometimes helps in rendering classical singularities interior submanifolds. In isotropy, there is again a single co-triad component $e \in \mathbb{R}$, $e^i_a = e \delta^i_i$, such that $a = |e|$. The classical singularity at $e = 0$ is then an interior point. In these variables, classical singularities are boundaries not simply by definition of the basic variables but only for classical evolution which breaks down at $e = 0$. For quantum dynamics, the extendability of states thus becomes testable.

In the Bianchi I model, however, we have $e^i \in \mathbb{R}$ such that $a_I = |e_I|$. While the two vanishing triad components of a Kasner solution would correspond to interior points, the diverging one implies that the classical singularity is still located at the infinite boundary of minisuperspace. A further reformulation alleviates this issue: we use a densitized triad $E^a_i = |\text{det}(e^i_a)| e^i_a$, with the triad $e^i_a$ inverse to $e^i_a$, $e^i_a e^i_a = \delta^i_i$. Then, the single densitized triad component $p \in \mathbb{R}$ satisfies $a^2 = |p|$ in isotropic models where the classical singularity $p = 0$ is still located in the interior. In anisotropic models we have three components $p^i \in \mathbb{R}$ related to the metric components by $a_I = \sqrt{|p^i p^j / p^k|}$ and cyclic. (There is a gauge transformation which changes the signs of any two components $p^i$ leaving the third fixed. Thus, only $\text{sgn}(p^1 p^2 p^3) = \text{sgn}\det E^a_i$ is physically distinguishable.) For a Kasner solution, $p^i \propto t^{1 - a_I}$ where $1 - a_I \geq 0$. All densitized triad components approach zero at an anisotropic classical singularity which is thus realized as an interior point [41].

Typical homogeneous singularities occur as interior points of the densitized triad space. This is also true for the Schwarzschild singularity [42] and employing the BKL conjecture one can assume that general inhomogeneous singularities relevant for cosmology and black holes may have the same behavior. Given a candidate for quantum evolution, the extendability of wave functions can then be studied in finite neighborhoods. The choice of variables thus matters for quantum hyperbolicity which may seem an unwelcome dependence on coordinatization. But it is not only the characterization of classical singularities where the choice of variables matters but also, and even more so, for the success of a chosen quantization scheme. This determines which kind of quantum dynamics can be used with a set of states represented on the space of metrics or triads. It is thus an appealing possibility that the formulation of quantum dynamics may put restrictions on the choice of basic variables in a form which may or may not allow one to realize quantum hyperbolicity. The structure of classical singularities then becomes an important means to test general issues of dynamics in quantum gravity in a way nicely intertwining classical relativity with quantum geometry and dynamics. We will discuss these issues in detail in the following sections.
FIGURE 10. Isotropic minisuperspace in densitized triad variables $p$ with a matter field $\phi$. Quantum hyperbolicity requires a unique extension of wave functions across the line $p = 0$.

3.4.3. Requirements on quantum dynamics

The quantum hyperbolicity principle is testable as it requires crucial properties of quantum dynamics to be realized. Continuations of wave functions are relevant and thus the mathematical type of dynamical equations. On the other hand, the principle is insensitive to conceptual issues such as the interpretation of wave functions, observables or evolution which are largely unresolved in quantum gravity. Progress can thus be made on the singularity issue even before quantum gravity is fully understood.

Using densitized triad variables in isotropic cosmology leads to a dynamical equation of the type

$$\Delta \psi(p, \phi) = \hat{H} \psi(p, \phi)$$

with a differential operator $\Delta$ on superspace and a matter Hamiltonian $\hat{H}$ which is usually a differential operator on the matter field also containing metric components. For quantum hyperbolicity we must be able, starting from suitable initial values at one side of $p = 0$ such as large positive $p$, to extend any solution uniquely across $p = 0$ as illustrated in Fig. 10.

Any matter Hamiltonian $H$ defined with a fundamental field rather than phenomenologically through an equation of state contains $p^{-1}$, such as in

$$H = \frac{1}{2} |p|^{-3/2} p_p^2 + |p|^{3/2} V(\phi)$$

for a homogeneous scalar with momentum $p_\phi$. The reason for this general behavior is that momenta in a relativistic canonical formulation carry a density weight. Since momenta appear in quadratic form in usual matter Hamiltonians, this requires an inverse of the determinant of the metric to get a well-defined, coordinate independent integration of the total Hamiltonian. This inverse determinant leads to $|p|^{-3/2}$ in an isotropic reduction. For a well-defined evolution interpretation of the equation in $p$, the coefficients in the diff. equation must not diverge especially at $p = 0$. This requires that a quantization taking into account gravity must lead to a matter Hamiltonian where the divergence of the kinetic term at $p = 0$ does not arise. One can interpret this as saying that quantum hyperbolicity in an isotropic model requires bounded curvature because classical curvature in an isotropic model behaves as an inverse power of the scale factor. This requirement is intuitively reasonable, but it is only secondary and derived from quantum hyperbolicity for isotropic models.

This bounded isotropic curvature condition is much easier to check than quantum hyperbolicity and thus provides an easily accessible indication of its realizability. For the Wheeler–DeWitt equation (in an ordering as it occurs, for instance, in [43, 44])

$$\frac{2}{9} \hbar^2 \frac{\partial^2}{\partial p^2}(\sqrt{|p|\psi(p, \phi)}) = \frac{8\pi G}{3} \left( \frac{\hbar^2}{2} |p|^{-3/2} \frac{\partial^2 \psi}{\partial \phi^2} - |p|^{3/2} V(\phi) \right) \psi(p, \phi)$$

(10)

with the ordinary quantization of $p$ as a multiplication operator the condition is obviously not satisfied: the right hand side diverges generically at $p = 0$. Then, even with the classical singularity being interior in densitized triad variables, there is a break-down of the initial value problem at $p = 0$. Wheeler–DeWitt quantum cosmology violates quantum hyperbolicity.

Discrete approaches provide simple solutions to this problem if the continuous $p$-space is replaced by a lattice not containing $p = 0$. Coefficients of the resulting difference equation are then never evaluated at $p = 0$ and no divergence arises. But as this avoidance of a singularity would merely be put in by hand by choosing a suitable lattice such a resolution would hardly seem satisfactory. (A more refined version of this possibility can be found in [45, 46].)

6 Recall that this means differential or difference.
As we will see later, quantizations which pass the bounded isotropic curvature test of quantum hyperbolicity do exist. Bounded curvature in isotropic models thus provides a simpler but non-trivial test of quantum hyperbolicity. It is, however, not to be over-generalized, as it has occasionally been done in the recent literature, as anisotropic models show. In anisotropic models the classical singularity occurs at $p^1 = p^2 = p^3 = 0$. This is a single point in the interior of 3-dimensional minisuperspace. Unlike the classical trajectory sketched in Fig. 11, a wave function will be supported on 3-dimensional regions. Coefficients of the dynamical equations then can become singular even if a single $p^i$ vanishes. All three planes $p^i = 0$ are thus to be considered potentially singular for quantum dynamics.

As before, coefficients of the diffusion equation must not diverge for a well-posed initial value problem. Again, the danger comes from a matter Hamiltonian but possibly also from intrinsic curvature which can diverge in anisotropic models. Now, however, boundedness is not required on the whole minisuperspace; only a local version in any finite subset of the singular hyperplanes is necessary. Curvature can (and usually does) grow parallel to singular submanifolds, e.g. for $p^1 \to \infty$ while $p^2$ and $p^3$ remain small. This shows that bounded curvature operators are not required in any non-isotropic model. An analysis of the singularity issue then has to refer to more detailed properties of quantum dynamics and the corresponding initial value problem.

This is also the case in any inhomogeneous model. In such cases, many coupled diffusion equations result, one for each spatial point as the equations are functional. Although equations remain linear, initial or boundary value problems are much more complicated and to be analyzed in detail. Without any symmetry it would not even be known how to locate classical singularities on superspace in a one-to-one manner. This complicates any scheme to resolve singularities, not just the principle of quantum hyperbolicity. Moreover, in full situations one may have to expect non-commutative metric operators to occur (see, e.g., [47, 48, 49]). This shows that bounded curvature operators are not required in any non-isotropic model. An analysis of the singularity issue then has to refer to more detailed properties of quantum dynamics and the corresponding initial value problem.

4. CANONICAL QUANTIZATION

To address the singularity issue from the point of view of quantum hyperbolicity, i.e. the unique extendability of states across classical singularities, a sufficiently detailed formulation of quantum dynamics is needed. Proper wave functions are required, independent of any background metric. Only then can quantum geometry be taken into account fullly which on smaller scales or close to a classical singularity can be very different from classical geometry. Canonical quantizations allow systematic constructions of quantum field theories even without reference to a background metric. The metric itself can then be a full quantum operator and, e.g., fluctuate. Its quantum dynamics is relevant for the singularity issue.

In canonical gravity, there is an infinite dimensional phase space, in ADM variables [52], of fields $q_{ab}$, the spatial metric, and momenta $p_{ab}$, related to extrinsic curvature. The other components $N$ and $N^a$ of the space-time metric (11) are not dynamical since $\dot{N}$ and $N^a$ do not occur in the action. Thus, according to the usual definition as the derivative of the action by time derivatives of fields, momenta $p_N$ and $p_{N^a}$ vanish identically. Rather than determining the evolution of $N$ and $N^a$, their equations of motion $0 = \dot{p}_N = -\frac{\delta H}{\delta N}$ and $0 = p_{N^a} = -\frac{\delta H}{\delta N^a}$ imply constraints on the phase space
variables: the Hamiltonian constraint
\[ 0 = \frac{\delta H}{\delta N} = \frac{\sqrt{\det g}}{16\pi G} (3) R - \frac{16\pi G}{\sqrt{\det g}} (p_{ab} p^{ab} - \frac{1}{2} (p^a_a)^2) \]

and the diffeomorphism constraint
\[ 0 = \frac{\delta H}{\delta N^a} = 2 D_b p^b_a. \]

For a generally covariant theory the total Hamiltonian is a sum of constraints since no preferred time variable exists to which absolute evolution generated by a non-vanishing Hamiltonian would refer. For general relativity, we have the Hamiltonian
\[ H = H[N] + D[N^a] = \int d^3x N(x) \frac{\delta H}{\delta N} + \int d^3x N^a(x) \frac{\delta H}{\delta N^a} \]
(11)

and the constraints determine the full dynamics. They constrain allowed values of the fields and their initial data, and they generate Hamiltonian equations of motion in coordinate time through Poisson brackets such as \( \{ q_{ab}, H \} \). On the right hand side of those equations of motion lapse and shift occur through \([11]\). For specific equations of motion, they thus have to be specified by choosing a space-time gauge. This determines which coordinate the dot in equations of motion refers to (e.g. proper or conformal time depending on whether \( N = 1 \) or \( N = a \) in isotropic cosmology).

This is different in quantum gravity since there will be no reference to the space-time coordinates at all. Dynamics must be described in a gauge-independent manner rather than using space-time coordinates. While this is also possible, though complicated, to do in classical gravity, in background independent quantum gravity it is the only option. The tensors \( q_{ab} \) and \( p^{ab} \) are then to be replaced by operators, acting on states such as \( \psi[q_{ab}] \) solving the infinitely many quantum constraints
\[ \hat{H}[N] \psi = \hat{D}[N^a] \psi = 0 \quad \text{for all } N \text{ and } N^a. \]

The difficult part is to define precisely which function space \( \psi[q_{ab}] \) refers to, how basic operators quantizing \( q_{ab} \) and \( p^{ab} \) are represented in a well-defined way, and how their products or even non-polynomial expressions in the constraints are being dealt with.

All these steps simplify in homogeneous models such as in isotropic Wheeler–DeWitt cosmology. Classically, \( q_{ab} = a^2 \delta_{ab} \) just requires a single variable \( a \) to be quantized without any tensor transformation laws to be taken care of in this restricted class of coordinates respecting the symmetry. Wave functions \( \psi(a) \) are simply square integrable functions of a single variable. The Wheeler–DeWitt equation is obtained by quantizing the Hamiltonian constraint:
\[ \frac{1}{a} \frac{\partial}{\partial a} \frac{\partial}{\partial a} a \psi \approx \hat{H}_{\text{matter}} \psi \]

where there is some freedom in choosing the operator ordering of \( a \) and \( \partial / \partial a \) (the ordering here agrees with \([10]\)).

The diffeomorphism constraint \( \hat{D} = 0 \) vanishes identically.

### 4.1. Index-free objects

In general, a well-defined background independent quantization is much more complicated due to, for instance, non-trivial transformation properties of tensorial basic variables. A single component \( q_{\mu\nu} \) does not have coordinate independent meaning, but only the tensor \( q_{ab} \) has. If we quantize single components, the question is which coordinate system an operator \( \hat{q}_{\mu\nu} \) should refer to. Properties of space are to be determined by states (e.g. through expectation values) only after operators have been defined. The space–time manifold in general relativity is part of the solution to Einstein’s equation, whose coordinates follow from coordinates on an initial spatial slice once the gauge has been fixed fully. Thus, it becomes available only after the classical constraint and evolution equations have been solved. In quantum gravity, we have to turn the basic tensors given by the spatial metric and its momentum into operators before we can even formulate the constraint equations. There is thus no meaning whatsoever to an operator “\( \hat{q}_{\mu\nu} \)” because its classical analog \( q_{\mu\nu} \), when defined in one chosen coordinate system, will receive factors \( \partial \chi^\mu / \partial x^\mu \) when transformed.
to other coordinates. (These coordinates are only spatial because a canonical formulation deals with spatial tensors. Nevertheless, the classical tensors transform in this manner on any spatial slice, not just the “initial” one.) One can certainly avoid this by choosing a fixed set of spatial coordinates on any slice once and for all. But the resulting quantum theory would keep a trace of that choice and would be badly non-covariant.

For this reason, no systematic quantization is known in ADM variables using the spatial metric and its momentum. No full quantum theory has been formulated in those variables but one has constructed exclusively models where one can reduce the metric variables to scalar quantities. Scalar quantities can then more easily be quantized since they do not receive coordinate dependent factors from the tensor transformation law. Examples include homogeneous models where the metric is determined by a finite number of spatial constants which do not transform under the allowed coordinate changes preserving the symmetry. (In fact, even such simple models can give rise to confusion from coordinate changes. An example is the scale factor of flat isotropic models which can be rescaled arbitrarily by a constant. This rescaling freedom cannot be appropriately dealt with in a quantization of the model unless the freedom is fixed from the outset.) Also in inhomogeneous models such as Einstein–Rosen or Gowdy models one can sometimes express the metric in terms of scalar fields on a given manifold \([53, 54]\). But those are special properties not available in a similar form in full generality. It then remains unclear if those quantum models show typical properties of quantum gravity or special features used in their formulation. In particular, there is no well-defined relation between those symmetric quantum models and a potential full theory.

To proceed, we thus need to reformulate unrestricted spatial geometries in terms of index-free objects. A successful classical reformulation starts by first removing one spatial index from \(q_{ab}\) and \(p^{ab}\) (or \(K_{ab}\)). As already used, we introduce the co-triad \(e^i\) such that \(e^i_a e^j_b = q_{ab}\). Here, \(i\) is just an index enumerating co-vectors and does not imply transformation properties under changes of coordinates. Moreover, the position of this index is irrelevant and will be summed over even when repeated in the same position. Similarly, we trade in an index \(i\) for a spatial index in extrinsic curvature by defining \(K^i_a := e^i_e K_{eb}\), using the triad, i.e. the inverse \(e^i\) of \(e_a\). We cannot proceed further in this way and remove all spatial indices because \(e^i_j e^j_a = \delta^i_a\) would loose all information about the metric. The triad, on the other hand, has all information about the metric. In fact, it has more freedom because an \(SO(3)\) rotation \(R^i_j e^j\) leaves the metric \(q_{ab}\) unchanged. This corresponds to the three additional components which the (non-symmetric) matrix \(e^i\) has compared to the symmetric \(q_{ab}\). The new degrees of freedom are removed from the resulting field theory by imposing a further constraint on triad variables which has the form of the Gauss constraint in an SU(2) Yang–Mills theory.

Using \(K^i_a\) as one of the canonical variables leads to a momentum which is not exactly the triad but its densitized version, the densitized triad \(E^i = |\det e^i_j| e^i_j\). At this point we should recall that densitized triad variables were very convenient for the singularity issue because they implied positions of classical singularities in the interior of the space of geometries. At this point we see how the choice of basic variables also plays a role when defining a quantum theory. As we proceed, we will see that a reformulation of classical gravity in terms of index-free objects is possible precisely in terms of variables which use the densitized triad instead of the spatial metric or co-triad.

To proceed with the definition of index-free objects, we will replace the tensor \(K_{ab}\) by a connection. This will immediately suggest an index-free object, a holonomy, and has the additional advantage that spaces of connections are much better understood mathematically than spaces of extrinsic curvature tensors or metrics. Just as the metric defines a Christoffel connection, the co-triad defines the spin connection

\[
\Gamma^e_a \equiv -e^j^b e^i^c (\partial_a e^j_b) + \frac{1}{2} e^j^b e^i^c \partial_a e^j_b.
\]

As a functional of \(e^j_b\), it has vanishing Poisson brackets with \(E^i\) and can thus not be used as a momentum replacing \(K^i_a\). But the Ashtekar connection \([55, 56]\) \(A^i_a = \Gamma^e_a - \gamma K^i_a\) transforms as a connection, as any sum of a connection and a tensor does, and is canonically conjugate to the densitized triad because \(K^i_a\) is. In the definition, \(\gamma > 0\) is the Barbero–Immirzi parameter \([56, 57]\) which does not have any effect in the classical theory but is important in quantum gravity.

Loop quantum gravity is based on a canonical quantization of the phase space spanned by \(A^i_a\) and \(E^i\) with

\[
\{A^i_a(x), E^j_b(y)\} = 8\pi G \delta^j_a \delta^i_b \delta(x, y).
\]

Its success relies on the fact that connections and densitized vector fields can easily be expressed in terms of index-free objects which can then be represented on a Hilbert space. Instead of connection components we use holonomies

\[
h_x(A) = \mathcal{P} \exp \int_c A^i_a x^a dt
\]
for curves $e$ with tangent vector $\dot{e}^i$ and Pauli matrices $\tau_j = -\frac{i}{2} \sigma_j$. As usually, $\mathcal{P}$ denotes path ordering along $e$ of the non-commuting functions in the integrand. If holonomies are known for all curves $e$ in space, the connection can be reproduced uniquely \[58\]. Similarly, we use fluxes

$$ F_S(E) = \int_S d^2y n_a E^a_i \tau_i $$

for 2-surfaces $S$ with co-normal $n_a = \frac{1}{2} e_{abc} \epsilon^{wm} \frac{\partial x^m}{\partial y^w} \frac{\partial x^c}{\partial y^e}$ in a parameterization $S: y \mapsto x(y)$. Again, if fluxes are known for all surfaces $S$ in space, the densitized triad is reproduced uniquely.

Notice that no background metric is used in these definitions as the tangent vector as well as co-normal are defined intrinsically without reference to a metric. Moreover, there are no free spatial indices and the objects transform trivially under changes of coordinates. Instead, there is a representation of active spatial diffeomorphisms $\phi$ which move along the labels $e \mapsto \phi(e)$ and $S \mapsto \phi(S)$ of holonomies and fluxes. These objects can thus be represented on a Hilbert space without having to include coordinate factors in the tensor transformation law.

### 4.2. Loop quantum gravity

For a representation one also has to know the Poisson algebra of basic variables which is to be turned into a commutator algebra. Poisson relations of holonomies and fluxes define the holonomy-flux algebra in which no delta functions occur even though we are dealing with a field theory: integrating connections and densitized triads to obtain index-free objects has automatically introduced the correct kind of smearing. Any delta function present in the Poisson relations are reproduced uniquely.

Notice that no background metric is used in these definitions as the tangent vector as well as co-normal are defined intrinsically without reference to a metric. Moreover, there are no free spatial indices and the objects transform trivially under changes of coordinates. Instead, there is a representation of active spatial diffeomorphisms $\phi$ which move along the labels $e \mapsto \phi(e)$ and $S \mapsto \phi(S)$ of holonomies and fluxes. These objects can thus be represented on a Hilbert space without having to include coordinate factors in the tensor transformation law.

#### 4.2.1. Representation

One can now construct a quantum representation of the smeared basic fields which arose naturally in providing variables suitable for a background independent quantization. After the basic objects have been represented, thus providing a quantum theory, one can quantize and impose constraints as operators. This will ensure that only space-time covariant observables arise. From the form of the basic variables, an SU(2) connection and a densitized momentum field in Ashtekar variables, general relativity appears as a gauge theory subject to additional constraints.

A representation is most easily constructed in the connection representation where states are functionals on the space of connections. This would not be available had we not been led to introduce connections rather than tensors in constructing index-free objects; the representation will thus carry characteristic features as traces of the background independent quantization. In a connection representation, holonomies act as multiplication operators. Starting from a basic state which, as a function of connections, is constant, we thus “create” non-trivial states which depend on the connection along the edges used in multiplicative holonomies. Although such states depend on the connection only along edges, the resulting states can be complicated with edges non-trivially being knotted and linked with each other. Moreover, edges can intersect each other giving rise to vertices in which more than two edges meet. The resulting space of states can be spanned by a basis of spin network states \[59\] defined as

$$ f_{g,j,C}(A) = \prod_{v \in g} C_v \prod_{e \in g} \rho_{j_e}(h_e(A)) $$

where $g$ is an oriented graph collecting all the edges used for holonomies, with labels $j_e$ indicating irreducible SU(2) representations $\rho_{j_e}$ in which edge holonomies are evaluated, and matrices $C_v$ which ensure that matrix elements of holonomies are multiplied with each other in a way resulting in a gauge invariant complex valued function of the
connection. Since holonomies are multiplied with SU(2) group elements at the endpoints of their edges under a gauge transformation, the contraction matrices sit in vertices where different edges meet each other.

A well-known example of a gauge invariant function of holonomies is the Wilson loop obtained by taking the trace of a holonomy around a closed loop. In the fundamental representation, we can reproduce this in the above language by introducing two vertices $v_1$ and $v_2$ along the loop which split the loop into two non-self-intersecting edges $e_1$ and $e_2$. We orient this graph such that both edges start in $v_1$ and end in $v_2$. Their holonomies in the fundamental SU(2) representation are $2 \times 2$ matrices $h_i(A_{ij})$ which change under a local gauge transformation to $g(v_1)^{ij}_D h_i(A) g(v_2)^{-1(j)}$ where $g(v_i)$ are the fundamental SU(2) are the values the local gauge transformation takes in the vertices. There are thus two factors in each vertex, such as $g(v_1)^{ij}_D h_1(A) g(v_2)^{-1(j)}$ from the two holonomies, which in the final expression must cancel each other when contracted with the matrix $C_{v_1}$. Using the identity $C_{v_1} = (g^{-1})(g)$ satisfied for any SU(2)-matrix $g$, one can see that a matrix $C(v_1) = e$ and similarly $C(v_2) = e$ results in a gauge invariant function: $C(v_1) g C(v_1) = C(v_1)(CD)$. The resulting spin network state

$$W(A) = e A e B D \cdot h_1(A) h_2(A)) g B = (h_1(A) h_2(A)) g B = (h_1(A) h_2(A))$$

leads to the usual expression for the Wilson loop, where in the second step we used the same SU(2) identity as before. At intersection points of higher valence, one can use decompositions of tensor products of SU(2) representations into irreducible ones, i.e. the usual recoupling rules known from angular momentum in quantum mechanics, to find all vertex matrices $C_v$ leading to gauge invariant results.

Spin network states span the whole quantum representation space because the action of holonomies as basic configuration variables is complete. On any such state, holonomies are represented as multiplication operators as used in the construction of the states. Since these operators have to respect unitarity properties representing the classical reality conditions of $A_{\mu}$, an inner product of the representation space results. In this process spin network states turn to be specific, that the surface intersects the edges at its starting point) gives

$$\int_S d^2 y \cdot \frac{\delta h_e}{\delta A_{\mu}(y)} = \frac{1}{2} \int_S d^2 y \int_e d\mu(y) e^2 \delta(e(t),y) h_e = \frac{1}{2} \text{Int}(S,e)$$

and thus a factor $\text{Int}(S,e)$ of the oriented intersection number of the surface $S$ and an edge $e$. Individual contributions in the sum over intersection points are then determined by "angular momentum operators" (su(2) derivatives)

$$\frac{\partial}{\partial h} \delta(h) = \text{tr}(\tau h \partial \delta / \partial h)$$

acting on holonomies. Since these operators have discrete spectra and are summed over in an at most countable sum, all flux operators have discrete spectra. With fluxes being the basic operators representing

FIGURE 12. A colored graph representing a spin network state together with a 2-surface intersecting a link.
spatial geometry through the densitized triad, discrete spatial geometry emerges from the construction without being put in in the first place.

This representation is not only convenient to construct and to work with, it is also, under mild assumptions, the unique representation of the algebra of holonomies $h_a$ and fluxes $F_S$ on which the diffeomorphism group acts unitarily $[60, 61, 62]$. Classically, diffeomorphisms $\phi$ act on holonomies and fluxes by moving the defining submanifolds, $(h_e, F_S) \mapsto (h_{\phi(e)}, F_{\phi(S)})$. If this is required to carry over to the quantum theory, as it should be since any violation of unitarity of the diffeomorphism group would imply a breakdown of spatial background independence, no other representation is possible. As it happens often, the requirement of a symmetry reduces the class of available representations. With the large diffeomorphism group as a consequence of background independence, the representation appears to be selected uniquely.

### 4.2.2. Quantum geometry

While fluxes do not have direct intuitive implications for spatial geometry, they occur in more typical objects such as the area operator. The area of a surface $S$ with co-normal $n_a$ as used in the definition of fluxes is $A(S) = \int_S \sqrt{g} \, n_a E_b^a n_b$. A quantization thus requires a product of flux operators which can be defined after regularization $[63, 64]$. Due to the square of triad components present in the classical expression, the quantum operator contains a square of angular momentum operators whose spectrum is well-known. This allows one to determine the area spectrum $\int_S \sqrt{E^a_b E^b_a}$.

\[
\hat{A}(S) f_{x_i} = \frac{1}{2} \gamma g^2 \sum_{p \in \mathcal{N} | g} \sqrt{J_p(j_p + 1)} f_{x_i}
\]

valid for the case where no intersections between $S$ and the graph occur in vertices of $g$. In the general case the spectrum is more complicated but also known explicitly.

Similarly, a volume operator $\hat{V}$ is obtained by quantizing the classical expression $V(R) = \int_R d^3x \sqrt{\det E}$. Again after regularization, contributions now come only from vertices $v \in R \cap g$ whose values are constructed from the invariant matrices in the vertex $[63, 65]$. Although the spectrum is much more complicated to determine than the area spectrum and not known completely, it is discrete.

The volume spectrum contains zero as a highly degenerate eigenvalue which is realized for instance, but not exclusively, in the case where no vertex lies in the region $R$. But also the total volume of the whole spatial slice has a highly degenerate zero eigenvalue even for vertices with arbitrarily high valence. Therefore, there is no densely defined inverse of $\hat{V}$. However, when we come to matter Hamiltonians we will need the inverse determinant of $E_i^j$, such as in the case

\[
H_\phi = \int d^3x \left( \frac{1}{2} \rho^2 + \frac{E^a_b E^b_a \partial_\alpha \phi \partial_\beta \phi}{\sqrt{\det E}} + \frac{\sqrt{\det E} V(\phi)}{\sqrt{\det E}} \right)
\]

of a scalar field. Since also metric components entering matter Hamiltonians have to be quantized in quantum gravity, we need an inverse volume operator. As the spatial volume vanishes usually at classical singularities, this issue is related to the singularity problem. In fact, in the context of quantum hyperbolicity we have already seen that such coefficients matter for the well-posedness of initial value problems of wave functions.

### 4.2.3. Quantization and ambiguities

Using

\[
\left\{ A^i_a, \int \sqrt{\det E} d^3x \right\} = 2\pi \gamma G \epsilon^{ijk} E_{ab} \frac{E^b_i E^c_j}{\sqrt{\det E}}
\]

and approximating $A^i_a$ by holonomies one can replace inverse powers of $\det E$ by positive powers in Poisson brackets $[66]$. Inserting holonomies and the volume operator, and replacing the Poisson bracket by $(\hat{h})^{-1}$ times a commutator then results in well-defined operators with a classical limit as required. But the resulting operators are not identical to an inverse volume which does not exist in the quantum theory. Deviations between the classical inverse and the quantum behavior thus result which are most noticeable at small length scales.
4.2.4. Dynamics

Also the constraints, in particular the Hamiltonian constraint

\[ H[N] = \frac{1}{16\pi G} \int_{\Sigma} d^3x N \left( \epsilon_{ijk} F_{i}^{a} E_{a}^{b} \frac{E_{k}^{b}}{\sqrt{|\det E|}} - 2(1 + \gamma^{-2})(A_{a}^{i} - \Gamma_{a}^{i})(A_{b}^{j} - \Gamma_{b}^{j}) \frac{E_{a}^{i} E_{b}^{j}}{\sqrt{|\det E|}} \right) \]

written in Ashtekar variables with \( F_{i}^{a} = 2\partial_{[i} A_{a}^{j]} + \epsilon_{ijk} A_{a}^{j} A_{b}^{k} \), are non-polynomial functions of the basic variables and thus subject to quantization ambiguities. But given the difficulties of other attempts to formulate quantum gravity, even a single well-defined quantization of the Hamiltonian constraint would be a success. With the techniques described before, this can be accomplished \cite{67,66}.

Also here, we need an inverse determinant of the triad which follows from the relation (17). We have not encountered the curvature components \( F_{i}^{a} \) before in operators, but they can be quantized by using the relation

\[ \Delta s_{1}^{a}s_{2}^{b} F_{i}^{a} \tau_{i} = \Delta^{-1}(h_{\alpha} - 1) + O(\Delta) \]

used also in lattice gauge theories. Here, \( \alpha \) is a square loop of coordinate size \( \Delta \) and with tangent vectors \( s_{1}^{a}, s_{2}^{a} \) in a vertex as shown in Fig. 13. One thus replaces the curvature components by holonomies around small loops which can then directly be represented on the Hilbert space. For this, one has to choose a prescription for the loops since the classical expression is simply evaluated in a point. The prescription gives rise to further quantization ambiguities which are, however, not as large as they would be for matter field theories on a background metric due to diffeomorphism invariance: only knotting and linking of the loop with edges in the graph of the state matters but not the precise position of an embedding in space.

The remaining terms in the constraint involve extrinsic curvature and are the most complicated to deal with. We would have to subtract the spin connection from the basic Ashtekar connection to obtain extrinsic curvature components. Ashtekar connection components could again be quantized using holonomies, but the spin connection (12) in general is a complicated function of the triad components. Moreover, it is not covariant, not even tensorial, and thus impossible to quantize directly. Instead of following this line it is conceptually easier to use a further identity \cite{66}

\[ K_{i}^{a} = \gamma^{-1}(A_{a}^{i} - \Gamma_{a}^{i}) \propto A_{a}^{i} \left\{ \int d^3x F_{i}^{a} \frac{e^{ijk} E_{j}^{a} E_{k}^{b}}{\sqrt{\det E}}, \int \sqrt{\det E} d^3x \right\} \]

which allows one to express extrinsic curvature through commutators of the already quantized first term in the constraint with the volume operator and holonomies. The result is a highly complicated operator, but it is well-defined. Moreover, it displays crucial properties and deviations from the classical behavior which can be studied in models where the operator simplifies.

4.2.5. Quantum effects

The typical properties shown by the construction of quantum Hamiltonians are results of using holonomies, the basic tenet of loop quantum gravity:

1. Quantized inverse powers of triad components give rise to modified small-scale behavior of coefficients. For singularities, this may be related to the issue of boundedness of coefficients in diff. equations as discussed before.
2. Replacing local curvature and connection components by holonomies along extended loops implies non-locality as well as higher order spatial derivatives. This will be seen later to imply difference operators in equations for wave functions.

In suitable semiclassical states, the quantum Hamiltonian must have an expectation value identical to the classical expression to zeroth order in \( \hbar \). In any interacting (non-linear) theory, however, there will be quantum corrections which one can formulate in effective classical equations as will be discussed in the final section. In deep quantum regimes, full quantum equations have to be used with potentially very different properties compared to classical behavior or the Wheeler–DeWitt quantization as we will study them in the next section. This provides a general framework for quantum dynamics in which quantum hyperbolicity is testable.

5. LOOP QUANTUM COSMOLOGY

Loop quantum gravity provides a non-perturbative and background independent formulation of quantum gravity. Its main ingredients are a well-defined representation of basic fields, spatial discreteness and candidates for quantum dynamics. A description to study singularities from the perspective of quantum gravity is thus in principle provided but, in such a general setting, difficult to apply. There are not just severe complications from technical as well as conceptual issues of quantum gravity, but already the classical understanding of singularities in general is not precise enough even to decide where one would have to look for resolved singularities in quantum gravity.

As in classical relativity, it is helpful in such a situation to study in detail explicitly treatable, usually symmetric situations where general aspects of quantum dynamics can be seen in action. This will at least give examples for singularity resolution and can suggest general mechanisms. By looking at different classes of models one then has a good chance of deciding whether or not such mechanisms are general or make use of special properties only realized in such models. Several unsuccessful examples are known, and also one so far successful scheme to be discussed here.

When using symmetric models in quantum gravity one should be aware of differences between classical symmetric solutions, which are exact albeit special solutions of full general relativity, and symmetric quantum models. In contrast to classical solutions symmetric quantum solutions cannot be exact since uncertainty relations are violated. Both the configuration variables (the densitized triad \( E_i^\alpha \)) and their momenta (the Ashtekar connection \( A_i^\alpha \)) must be symmetric to ensure a space-time solution respecting the symmetry everywhere. Non-symmetric modes of all canonical variables are thus zero which is possible classically but not in the presence of quantum uncertainty relations. A more general stability analysis is then required which has been done in a few cases. Alternatively, one can relax symmetries once models are well-understood and try to approach the full situation as closely as possible.

An additional aspect of loop quantum gravity makes symmetric models worthwhile and shows that they can capture essential ingredients of a full quantization of gravity. Models can in particular illustrate consequences of quantum representations which have wide implications not only for the basic variables represented but for any composite operator constructed from them. The full representation induces distinguished representations of basic variables (analogously to holonomies and fluxes) in symmetric sectors which, at a kinematical level, are thus derived from the full theory \([68]\). Since the full representation is unique, the induced representations of models are distinguished among all representations one could try in a mini- or midisuperspace quantization.

The induction proceeds by first identifying symmetric states in the full setting \([69]\). This is possible in a distributional sense, although the underlying discrete structure prevents the existence of any non-trivial normalizable state invariant under a continuous symmetry. The induced representation is then derived through basic full operators fixing these states, determining the reduced Hilbert space structure as well as the action of reduced basic operators (see the corresponding sections in \([70,71,72]\)). Composite operators then are to be constructed from those basic ones within the model following the same steps as in a full setting. A derivation from full composite operators would be more complicated and has so far not been attempted. But for testing properties of the basic loop representation the sketched procedure is sufficient. After all, dynamics has not been defined uniquely in the full theory and even an unambiguous derivation of the Hamiltonian constraint of a model from a full candidate would thus not result in a unique quantum dynamics. The situation in models is thus the same as that in the full theory where several candidates for dynamics formulated on a distinguished representation exist. The only difference is that models are often treatable explicitly and thus allow one to check physical consequences of different proposals for dynamics. In this way, the theory becomes physically testable.

Models allow one to understand the full theory because its characteristic properties are preserved during the induction procedure. Most importantly, discreteness of spatial geometry is realized in an analogous way as we will
see soon. Thus, even in isotropic models the representation is inequivalent to the Wheeler–DeWitt one which would have a continuous spectrum of the scale factor as a multiplication operator on the positive real line. This is the key reason why loop quantum cosmology, as the theory of symmetric sectors of loop quantum gravity is called, provides new insights even for the extensively studied field of quantum cosmology.

In addition to the fact that quantum dynamics is often treatable explicitly in models, there is the added advantage of a much clearer classical singularity structure. In isotropic models, for instance, for the usual matter ingredients it suffices to formulate the condition \( \alpha = 0 \) to select singular states, which is easily done using the volume operator. Direct tests of quantum hyperbolicity then become possible.

### 5.1. Isotropic models

The basic quantities of an isotropic model formulated in Ashtekar variables comprise one conjugate pair \((c, p)\) with

\[
|p| = \frac{1}{4} a^2 , \quad c = \frac{1}{2} (k + \gamma \dot{a}) .
\]  

(19)

The only difference to metric variables is the fact that \( p \) can take both signs since it describes a densitized triad. The sign of \( p \) then is the intrinsic orientation of space. The parameter \( k \) in \( c \) is \( k = 0 \) for a spatially flat model and \( k = 1 \) for positive spatial curvature. For negative spatial curvature the connection has a different form not covered here (see \([74]\)).

The induced quantum representation must be a quantization of this finite dimensional model. However, it differs from the usual Schrödinger representation one would use in a Wheeler–DeWitt quantization. A complete set of orthonormal states is given by \([75]\)

\[
|c\rangle = e^{i\mu c/2} , \quad \mu \in \mathbb{R}
\]  

(20)

which already demonstrates the inequivalence to usual quantum mechanics where plane waves would not be normalizable. Moreover, the Hilbert space is non-separable, i.e., has an uncountable basis. Basic operators, obtained by full flux and holonomy operators fixing the symmetric states (20) interpreted as distributions, act on these states by

\[
\hat{\rho} |\mu\rangle = \frac{1}{8} \gamma^2 \hat{\rho}^2 |\mu\rangle , \quad e^{i\mu c/2} |\mu\rangle = |\mu + \mu'\rangle .
\]  

(21)

These operators indeed demonstrate the same properties we saw in the full theory: \( \hat{\rho} \) has a discrete spectrum since all its eigenstates \( |\mu\rangle \) are normalizable, and \( e^{i\mu c/2} \) is represented but not \( c \) itself which is the hallmark of any loop representation. (It is not possible to derive a \( c \)-operator by taking a derivative by \( \mu' \) because the matrix elements of \( e^{i\mu c/2} \) in the basis states are not differentiable.) There is only a difference in how the discreteness of the spectrum of geometrical operators such as \( \hat{\rho} \) is realized since the set of all eigenvalues of \( \hat{\rho} \) is the whole real line. Nevertheless, the operator has a discrete spectrum since all its eigenstates are normalizable. In usual quantum mechanics, with a separable Hilbert space, this would imply that the set of eigenvalues is a discrete subset of the real line. On a non-separable Hilbert space as we have it here with an uncountable basis labeled by \( \mu \in \mathbb{R} \), however, an operator with a discrete spectrum can have any eigenvalue set. We will later see that the mathematical definition using normalizability of eigenstates is the one that is also relevant for the singularity issue. It is thus crucial that this property, rather than any statement about the set of eigenvalues, is preserved. This is a consequence of strong restrictions in the full theory from background independence and the subsequent transfer of the representation to symmetric models.

#### 5.1.1. Difference equation

With the induced representation, we can follow most of the steps done in full to construct Hamiltonian constraint operators. The classical Hamiltonian constraint with contributions from a matter Hamiltonian \( H_{\text{matter}} \) is

\[
H = -\frac{3}{8\pi G} \left[ \gamma^{-2}(c - k/2)^2 + k^2/4 \right] \sqrt{|p|} + H_{\text{matter}}(p, \varphi, \varphi\varphi) = 0
\]  

(22)

which can easily be seen to reduce to the Friedmann equation (with energy density \( \rho = |p|^{-1/2} H_{\text{matter}} \)) once \( c \) and \( p \) are replaced in terms of \( a \) and \( \dot{a} \) using \([19]\). This expression needs to be quantized by using “holonomies” \( e^{i\mu c/2} \), with some \( \mu_0 \in \mathbb{R} \) to be chosen, for the connection components and Poisson brackets for the triad components.
the latter part is not necessary since there is no inverse of $p$ due to cancellations from isotropy, we keep this step in order to have the quantization as close to the full one as possible.) The action of the resulting operator\footnote{There are different versions of this operator in the literature, which partially reflects the freedom existing in the full theory as well as details of the reduction to isotropic models which have not fully been worked out yet. For instance, one may reorder the operator, the one written here being non-symmetric, or include several effects which may be expected in an inhomogeneous quantization \cite{124,126}. We will mention these possibilities here only when they are relevant for the singularity issue.} can be determined explicitly, choosing $\mu_0 = 1$:

$$(\hat{H} - \hat{H}_{\text{matter}})(\mu) = \frac{3}{16\pi G\gamma^2 \ell_p^2} (V_{\mu+1} - V_{\mu-1})(e^{-ik}|\mu + 4) - (2 + k^2\gamma^2)|\mu + 4\rangle + e^{ik}|\mu - 4\rangle$$ (23)

with the quantized matter Hamiltonian $\hat{H}_{\text{matter}}$. In semiclassical regimes extrinsic curvature is small, $c - k/2 \ll 1$, which by construction leads to the correct classical limit even though exponentials of $c$ have been used.

The operator equation $\hat{H}\psi = 0$ to be solved for physical states can be expressed as a set of equations for expansion coefficients $\psi_\mu(\varphi)$ in $|\psi\rangle = \sum_\mu \psi_\mu(\varphi)|\mu\rangle$ which represent the state in the triad rather than connection representation. Applying the operator to such a general state and comparing coefficients of $|\mu\rangle$ results in the difference equation

$$(V_{\mu+5} - V_{\mu+3})e^{ik}\psi_{\mu+4}(\varphi) - (2 + k^2)(V_{\mu+1} - V_{\mu-1})\psi_{\mu}(\varphi) + (V_{\mu+3} - V_{\mu-3})e^{-ik}\psi_{\mu-4}(\varphi)$$ (24)

for $\psi_{\mu}(\varphi)$ written in terms of volume eigenvalues $V_\mu = (\gamma^2|\mu|/6)^{3/2}$ entering through commutators of holonomies with the volume operator.

This defines the dynamical equation for wave functions on minisuperspace, which can be applied now especially in a neighborhood of the classical singularity at $\mu = 0$ in the interior. There are two sides to the classical singularity thanks to the triad orientation. The key question then is whether quantum propagation stops at $\mu = 0$ as the classical evolution would at $p = 0$. We have the matter Hamiltonian in a coefficient of the difference equation, which must be well-defined at $\mu = 0$. This is our first test implied by quantum hyperbolicity in isotropic models as depicted in Fig.10.

The matter Hamiltonian $H_\varphi = \frac{1}{2}[p, e^{-3/2}p^2 + |p|^{3/2}V(\varphi)]$, as before, contains $p^{-3}$ which cannot be quantized directly since $p$ has a discrete spectrum containing zero and thus lacks a densely defined inverse.

5.1.2. Isotropic curvature bounds

This is the place where the definition of a discrete spectrum through the normalizability of eigenstates is key since this, rather than properties of the set of eigenvalues other than zero being contained in the set, implies the non-existence of an inverse operator. It thus seems that the situation is even worse than in a Wheeler–DeWitt quantization since coefficients in the matter Hamiltonian appear impossible to define at all. But classically, $a^{-3}$ can be rewritten in a form suitable for quantization, mimicking the full identity \cite{117} of \cite{120}, as

$$a^{-3} = \frac{3}{8\pi \gamma G l_j (j+1)(2j+1)} \sum_{j=1}^{3} \text{tr}(\tau_i h_i \{h_j^{-1}, |p|\})^{3/(2-2\ell)}$$

using only positive powers of $p$ and “holonomies” $h_i = e^{\tau_i}$. All this can directly be quantized, with the Poisson bracket becoming a commutator. Rewriting in this way introduces ambiguities because it can be done in many classically equivalent ways. Making different choices does, however, influence the quantization. Here, we have indicated two possibilities, taking different powers of $V$ in the Poisson bracket or taking the trace in different representations. Eigenvalues of the resulting operators can be computed explicitly,

$$\hat{d}(a)^{(j,l)}_{\mu} = \left(\frac{9}{\gamma^2 l_j l_j (j+1)(2j+1)} \sum_{k=-j}^{j} k |p_{\mu+2k}|^l \right)^{3/(2-2\ell)}$$ (25)

showing the dependence on the parameters $j$ and $l$.\footnotetext{There are different versions of this operator in the literature, which partially reflects the freedom existing in the full theory as well as details of the reduction to isotropic models which have not fully been worked out yet. For instance, one may reorder the operator, the one written here being non-symmetric, or include several effects which may be expected in an inhomogeneous quantization \cite{124,126}. We will mention these possibilities here only when they are relevant for the singularity issue.}
Despite of the ambiguities, there are crucial common properties to all these quantizations. The divergence of the classical $a^{-3}$ is cut off by quantum effects which is clear from the fact that the operator is well-defined on all basis states, even on $|0\rangle$ which corresponds to the classical singularity \[77\]. The expression for eigenvalues shows that inverse scale factor operators in fact all annihilate this state, irrespective of $j$ and $l$, since for $\mu = 0$ one is summing an odd expression in $k$ from $-j$ to $j$. One can most easily see the behavior around $\mu = 0$ by looking at an approximation of the eigenvalues valid for larger $j$. Viewing the sum as a Riemann sum of an integral, one obtains \[78\]

$$d(a)^{(j,l)} = d(a)_{\mu(a^2)} = a^{-3} p_l(3a^2/jy)^{3/(2-2l)}$$

with $\mu(p) = 6p/\gamma L^2$ and

$$p_l(q) = \frac{3}{27} q^{1-l} \left( \frac{1}{2} + \frac{1}{l+2} \left[ (q+1)^{l+2} - |q-1|^{l+2} \right] - \frac{1}{l+1} q \left( (q+1)^{l+1} - \text{sgn}(q-1)|q-1|^{l+1} \right) \right).$$

Important properties, i.e. the approach to classical behavior at large $\mu$, the peak at small values and the approach to zero for $\mu = 0$ are all robust as can be seen from Fig. 14 \[78\]\[79\].

5.1.3. Isotropic quantum hyperbolicity

The difference equation \[24\] for $\psi_\mu(\varphi)$ can be used to investigate quantum hyperbolicity in isotropic models. We have already seen that the coefficients remain well-defined even at $\mu = 0$. But this is only one first test which is necessary for quantum hyperbolicity to have a chance of being realized. We must, most importantly, be able to extend any wave function uniquely across $\mu = 0$. For this, the recurrence scheme determined by the difference equation must be well-defined, i.e. we must be able to compute $\psi_\mu$ from the preceding values which themselves have been computed from some initial values at large $\mu$. By following this procedure step by step one can see that evolution does continue from either side of the classical singularity (at $\mu > 0$, say) to a new branch (at $\mu < 0$) preceding the big bang at $\mu = 0$. This scheme with two sides to a classical singularity is provided automatically by ingredients we were forced to assume in loop quantum gravity \[80\]. It is, in contrast to bounded curvature which was a condition only in isotropic models, a general scheme which is even realized in inhomogeneous models. Since we know the geometrical meaning of $\text{sgn}(\mu)$ which changes during the transition through the classical singularity, we can interpret the process as a change in orientation: the universe turns its inside out. By restricting variables to metrics one completely misses this possibility of non-singular behavior, but also the precise form of quantum dynamics is necessary for a well-defined transition. Around $\mu = 0$, discreteness manifest in the difference equation is essential and classical space-time as a smooth manifold dissolves.

The penetration of the classical singularity is thus non-trivial despite the discreteness: $\mu = 0$ is contained in the lattice and not simply jumped over. Moreover, leading coefficients of the difference equation may vanish, which could imply a break-down of the recurrence. In a backward evolution, for instance, we solve recursively for $\psi_{\mu-4}$ in terms of $\psi_\mu$ and $\psi_{\mu+4}$. This is only possible if $V_{\mu-3} - V_{\mu-5}$, the coefficient of $\psi_{\mu-4}$ in the difference equation, is nonzero. But
it does vanish for $\mu = 4$ since $V_\mu$ depends only on $|\mu|$. The value $\psi_0$ of the wave function at the classical singularity thus appears to remain undetermined.

Nonetheless, $\psi_\mu$ is determined uniquely for all positive and negative $\mu$: $\psi_0$ just decouples completely. We can follow the recurrence to negative values of $\mu$. When determining $\psi_{-4}$, $\psi_0$ seems necessary. But it drops out of the equation because then the coefficient $V_1 - V_{-1}$ vanishes as well as the matter Hamiltonian which, as a robust property despite of quantization ambiguities, annihilates the state $|0\rangle$. The singular state $|0\rangle$ is then called *mantic* with respect to the given evolution: It plays a passive role in the recurrence scheme of quantum evolution. In general, a mantic states can be defined as one at which the recurrence scheme implied by the Hamiltonian constraint in the triad representation changes its form.

Mantic states have implications not just for the discussion of recurrence schemes, but they also imply *dynamical initial conditions* [81, 82]: Rather than determining $\psi_0$ which completely dropped out of the equations, the equation for $\mu = 4$ implies a linear relation between $\psi_4$ and $\psi_0$ and thus an additional linear relation between initial values chosen at large $\mu > 0$. There are thus restrictions on initial values not independent of but implied by the dynamical law, unlike the situation in every other area of physics. This implication, however, is more sensitive to the precise form of the constraint. Such conditions would be weaker for a symmetric ordering of the operator.

### 5.2. Anisotropic quantum hyperbolicity

As isotropic models are always very special, we have to drop symmetry conditions and see what remains of the observed mechanism of singularity removal. We first drop one of the isotropy conditions and look at space-times which are homogenous but have only one rotational symmetry axis. Such models are interesting for cosmology, but also for black hole physics since the interior inside the horizon of the Schwarzschild space-time is of this form.

The densitized triad for the Schwarzschild interior can be written as

$$E^\mu_\nu \partial \frac{\partial}{\partial x^\nu} = p_c \tau_1 \sin \vartheta \frac{\partial}{\partial \vartheta} + p_b \tau_2 \sin \vartheta \frac{\partial}{\partial \varphi} - p_b \tau_1 \frac{\partial}{\partial \phi}$$

in spherical coordinates where factors of $\sin \vartheta$ arise due to the density weight of $E_\mu^\nu$. There are now two independent triad components, $p_c$ and $p_b$. The determinant of the triad is $\det(E^\mu_\nu) = p_c p_b^2$ and its orientation $\text{sgn} p_c$ is solely determined by the sign of $p_c$. The sign of $p_b$ is irrelevant, and in fact there is a residual gauge transformation $p_b \rightarrow -p_b$ left after partially fixing the SU(2)-gauge by requiring the $x$-component of the triad to point in the su(2)-direction $\tau_3$ as used above.

The triad determines a spatial metric

$$\text{d}s^2 = \frac{p_b^2}{p_c} \text{d}x^2 + |p_c| \text{d}\Omega^2$$

whose comparison with the interior Schwarzschild metric ($r < 2m$ in the Schwarzschild coordinate where $r$ becomes time-like and is called $t$ in what follows), $\text{d}s^2 = (2m/t - 1) \text{d}x^2 + t^2 \text{d}\Omega^2$, allows us to identify the classical singularity on minisuperspace $(p_b, p_c)$: $p_c = 0$ at the Schwarzschild singularity while $p_b = 0$ is not a singularity but the horizon.

This model is loop quantized by a representation $\hat{p}_0 |\mu, \nu\rangle = \frac{1}{2} \sqrt{\gamma^2} \hat{\gamma}_0 |\mu, \nu\rangle$, $\hat{p}_c |\mu, \nu\rangle = \gamma^2 \hat{\gamma}_1 |\mu, \nu\rangle$ of basic triad operators acting on orthonormal states $|\mu, \nu\rangle$ with $\mu, \nu \in \mathbb{R}$, $\mu \geq 0$. As in isotropic models, one can write the Hamiltonian constraint equation for states as a difference equation (using $\psi_\mu = \psi_{-\mu}$) [83]

\begin{align}
2(C_{\mu+2} \sqrt{|\nu+2|} + C_\mu \sqrt{|\nu|}) \psi_{\mu+2, \nu+2} & - 2(C_{\mu-2} \sqrt{|\nu+2|} + C_\mu \sqrt{|\nu|}) \psi_{\mu-2, \nu+2} \\
+ (\sqrt{|\nu+1|} - \sqrt{|\nu-1|}) (\mu + 2) \psi_{\mu+4, \nu} & - 2(1 + 2\gamma^2) \mu \psi_{\mu, \nu} + (\mu - 2) \psi_{\mu-4, \nu} \\
+ 2(C_{\mu+2} \sqrt{|\nu-2|} + C_\mu \sqrt{|\nu|}) \psi_{\mu+2, \nu-2} & - 2(C_{\mu-2} \sqrt{|\nu-2|} + C_\mu \sqrt{|\nu|}) \psi_{\mu-2, \nu-2} = 0
\end{align}

where $C_\mu = |\mu + 1/2| - |\mu - 1/2| = \text{sgn}\mu$.

By the same procedure as before we conclude that this recurrence is singularity free which would also be realized if a matter term were present. Now, however, a more non-trivial test results: there are two boundaries of a metric minisuperspace, the horizon at $\mu = 0$ and the classical singularity at $\nu = 0$. Only one direction ($\nu$) is to be extended

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9 "MANTO: I stand still, around me circles time." Goethe’s Faust
in densitized triad variables if the singularity is removed. But there should be no extension through the boundary corresponding to the horizon because the validity of the homogeneous model breaks down outside the horizon. There is thus a non-trivial consistency check of the scheme: evolution through the classical singularity, but not the horizon must be realized. As one can see from the difference equation, the extension is provided in just the right manner. By the general scheme, wave functions are extended only from one orientation of the triad to another, which provides the new branch at the other side of the classical singularity. Since orientation is determined by $\text{sgn}(p_c)$, only the boundary at $p_c = 0$ is penetrated, which corresponds to the classical singularity. The horizon $p_h = 0$, on the other hand, remains a boundary even for quantum evolution. That this is indeed non-trivial can be seen by trying to reproduce the scheme in co-triad or triad variables without the density weight. Although there is a new branch of the opposite orientation, the position of singularities and horizons in minisuperspace is different and no natural singularity resolution follows.

5.2.1. Beyond the singularity

In general, solutions to difference equations, especially those of higher order as encountered in (24) and (27), could be wildly oscillating, such as $\psi_\mu = (-1)^\mu$ as a solution of $\psi_{\mu+2} - 2\psi_\mu + \psi_{\mu-2} = 0$. Wave functions could thus be sensitive to Planck scale physics even in large volume or small curvature regimes where classical physics should be a good approximation. Even if initial values in a semiclassical regime are chosen to avoid this, oscillations could develop after evolving through a classical singularity. This would make it difficult to interpret the new branch as a classical one even if it extends to large volume. Moreover, oscillating solutions of difference equations can even be growing exponentially in amplitude and thus dominate any non-oscillating part. That this does not happen is a restrictive stability condition [85] which happens to be satisfied automatically in isotropic models as presented above.

For the Schwarzschild interior, mantic states again play an important role for this issue. The coefficient $\psi_{2,0}$ of the wave function at $\mu = 2$, $\nu = 0$ drops out of the higher order term, which implies the symmetry of solutions under $\nu \mapsto -\nu$ [84]. If initial values at $\nu > 0$ are chosen so as to suppress oscillations on small scales (giving a so-called pre-classical wave function), oscillations will not arise at the other side. This is in accordance with staticity we know is realized in the outside region of Schwarzschild: there should be no difference between the past and the future of the classical singularity. It is again highly non-trivial how this is realized here through mantic states around the classical singularity in minisuperspace, although only the interior is used which itself is not static. But the classical interior dynamics is determined by the same constraint as the outside, just restricted to the interior variables. Although the quantum dynamics used here is not derived from an inhomogeneous constraint but constructed within the model mimicking the construction of the full constraint, we arrive at quantum solutions in accordance with the classical expectation. The dynamics is responsible for the symmetry of solutions which was not required at the kinematical level, in agreement with the static outside as it is determined by the classical constraint.

So far, it is unclear what happens in an inhomogeneous treatment of the black hole or with matter terms which would imply back-reaction on the geometry and non-trivial classical dynamics. A possible scenario concerning the information loss issue, based on several assumptions but taking into account singularity removal, has been described in [87]. Although suitable constraint operators and difference equations are available [88], they are very complicated to analyze. Some results are reviewed in [89, 90].

Oscillations of solutions are also related to the normalizability of wave functions in an inner product. States not only have to solve the difference equation but, as in any quantum theory, must be normalizable. This is not always obvious to do when implementing a quantum constraint which usually changes the inner product on its solution space. In our discussion so far, and for most of the rest of this section, we can safely ignore this issue since we were able to show that all solutions are uniquely extended across classical singularities. This must then also be true for the physically normalizable ones. Here we see that it is important to show that all solutions, not just “generic” ones, are extended.

Nevertheless, for more precise pictures of the evolution through a classical singularity knowledge of properties of the physical inner product can be relevant. One method to derive the inner product is group averaging [91] which can be understood as writing quantum solutions to the constraint $\hat{H}\psi = 0$ as $\delta(\hat{H})|\psi\rangle = \int d\mu \exp(i\mu)\psi$. This is difficult to compute for the constraints we have to deal with here (especially due to the absolute value around $\mu$ which prevents the use of Fourier transformations, see e.g. [22] for possible alternatives). But since $\hat{H}$ depends on momenta, its exponential is related to a shift operator in $\mu$. This suggests that normalizable states are indeed nearly constant on small scales and do not show strong oscillations. This justifies the condition of pre-classicality which has been introduced on intuitive physical grounds [81]. Oscillations only arise on larger scales where the matter term becomes important, or on smaller scales when curvature itself is large. Since, as we saw, pre-classicality can always be achieved...
locally by choosing suitable initial conditions, but may be difficult to achieve on both sides of a classical singularity, strong restrictions on the quantization can be expected from a consistent physical normalizability.

5.2.2. Unbounded curvature

In anisotropic models, intrinsic curvature terms or the matter Hamiltonian occur in coefficients of the difference equation and must be well-defined everywhere for a consistent recurrence scheme. As seen before, in isotropy this implied finite inverse volume if quantum hyperbolicity is realized, but it is a very special case. Indeed we have a more general behavior in anisotropic models. Non-isotropic quantum hyperbolicity does not require boundedness of curvature in this sense, and it is indeed not realized generally as can be seen from Fig. 15.

But as we saw, the recurrence relations still do not break down at classical singularities and quantum hyperbolicity is realized. Bounded curvature on all of minisuperspace is thus not required for quantum hyperbolicity. In loop quantum gravity, unboundedness occurs in such a way that it does not prevent quantum hyperbolicity [51].

5.3. Inhomogeneous models

In inhomogeneous models we have not just one constraint equation but infinitely many ones since the Hamiltonian constraint has to be satisfied for any lapse function. Moreover, these are coupled equations although, for a wave function $\psi$, they remain linear. For a spherically symmetric model, we have states

$$|\psi\rangle = \sum_{\vec{k}, \vec{\mu}} \psi(\vec{k}, \vec{\mu}) \vec{\mu}^{-k} \vec{k} \cdot \vec{\mu} \cdots$$

(28)

with labels $k_\epsilon \in \mathbb{Z}$ for the edges and $0 \leq \mu_\nu \in \mathbb{R}$ for vertices. Again using a triad representation, coefficients of the wave function are subject to coupled difference equations (one for each edge)

$$\hat{C}_0(\vec{k}) \psi(\ldots, k_-, k_+ + 2, \ldots) + \hat{C}_R(\vec{k}) \psi(\ldots, k_-, k_+ - 2, \ldots) + \hat{C}_L(\vec{k}) \psi(\ldots, k_+, k_+ + 2, \ldots) + \hat{C}_L^{-1}(\vec{k}) \psi(\ldots, k_-, k_+ + 2, \ldots) = 0$$

(29)

on an extended superspace of densitized triads. All coefficients $\hat{C}_i(\vec{k})$ are operators on the vertex labels $\mu$ which we suppressed in the notation. They have all been computed explicitly in [88]. Local orientation $\text{sgn} \det E$ is determined by $\text{sgn} k_\epsilon$ such that we have to investigate the behavior of the coupled difference equations around vanishing edge labels.
Again, evolution is non-singular [42] which here depends crucially on the form (especially possible zeros) of coefficients \( \hat{C}_{R\pm}(\vec{k}) \) in a way which is much more non-trivial than in isotropic models. Unlike in homogeneous models, a symmetric ordering is required to extend solutions. Still the solution space is restricted by dynamical initial conditions as a consequence of mantic states. This shows that extending models to include more degrees of freedom does lead to tighter conditions on the allowed quantizations. So far one scheme is working in all situations considered, a highly non-trivial result given the complexity of equations such as (29) compared to the much simpler case of (24).

### 5.4. General properties

The preceding examples exhaust all types of models where triad representations exist and which are so far treatable explicitly. They allow possible general considerations: assuming singularities of BKL-type, only homogeneous behavior and diagonal metric or triad components are essential close to most interesting classical singularities. This would imply the existence of a triad representation at least for good approximations also around general singularities where the above arguments discussed in models would go through. That neither inhomogeneities nor local degrees of freedom by themselves spoil quantum hyperbolicity in loop quantum gravity follows from the demonstration that spherically symmetric and polarized cylindrically symmetric models respect the mechanism [42, 88].

If this is not realized, non-commuting triad operators have to be taken into account. Metric components would thus be unsharp and the singularity appears washed out. An example realized in loop quantum gravity, as a consequence of non-Abelian SU(2)-holonomies, is discussed in [51]. While \( \delta(a) = a^{-3} \) used in [25] has the same eigenstates as \( \dot{a} \) or the volume operator \( \dot{a}^3 \), this is not the case if full SU(2) holonomies rather than U(1) elements \( e^{i\mu/2} \) are used. Using the basic equation (17), an inverse power is replaced by

\[
e^\mu \{ A'_\mu, V \} \approx 2e^{-1}\text{tr}(\tau h_e \{ h_e^{-1}, V \})
\]

with a holonomy \( h_e \) for some suitable edge \( e \) whose tangent vector is \( e^\mu \) and whose parameter length is \( \varepsilon \). The right hand side is a good approximation for small \( \varepsilon \) or small \( A'_\mu \), which allows one to expand the exponential of the holonomy. The left hand side is not connection dependent, despite its appearance, since the derivative in the Poisson bracket removes \( A'_\mu \). For holonomies \( h_e \) taking values in an Abelian group, the right hand side is also connection independent since the two holonomies cancel each other even after taking a derivative by connection components. But due to non-commutativity, the cancellation is not complete for non-Abelian holonomies. Thus, the right hand side, which is used directly for a quantization, does become connection dependent. As a consequence, the resulting operator will not commute with the volume operator even though the classical expression does not depend on momenta of the densitized triad.

This may lead to unsharp definitions of degeneracy points since it depends on which operator is used to determine eigenstates. There must be additional dynamical arguments to select the appropriate operator and its eigenstates as corresponding to classical singularities. Such situations would be much more complicated to analyze both from the classical perspective (structure of singularities) and for quantum dynamics. Fortunately, every indication so far, relying on dynamical properties of quantum gravity, points to properties as they were anticipated from models [51].

As we saw, symmetric models allow explicit investigations of many properties expected for singularities. It is important to keep a wide view of all types of characteristic models since any given model by itself may be too special as one can see it in isotropy. Still, there may always be properties not seen so far which may become relevant. According to the current status, quantum hyperbolicity is realized in much more general terms than any other mechanism to remove classical singularities. Moreover, it is suggested naturally by the structure of background independent quantum gravity (e.g. properties of singularities in densitized triads or the form of difference operators). Also the non-perturbative treatment matters, as shown in [70] where an anisotropic model was loop quantized not as described before but as a perturbation around a loop quantized isotropic model. Then, quantum hyperbolicity was not realized, in contrast to the full, non-perturbative quantization of the same model. Generalizations to less symmetric models have thus presented many non-trivial tests of the whole framework which so far were all passed successfully. A further test is the independence of the mechanism from details of the matter Hamiltonian, implying that we are dealing with a pure quantum geometry effect. Even curvature couplings, which can arise for non-minimally coupled scalar fields, do not change the mechanism [93] although at first the classical structure seems to be quite different from that in the absence of curvature couplings. The deep quantum picture crucially relies on spatial discreteness and dynamical equations for a wave function. This prevents detailed intuitive formulations, which in semiclassical regimes are sometimes available.
based on effective theory. Under certain conditions this can be applied to the transition through classical singularities, resulting in bounce pictures to be discussed in the next, final section.

6. SEMICLASSICAL PICTURES

As the general scheme of quantum hyperbolicity turns out to be realized in many cases in loop quantum gravity without counterexamples so far, it becomes possible to ask more detailed questions about the transition through classical singularities and in particular as to what happened before the big bang. The general mechanism utilizes in an essential way the discreteness of spatial geometry realized by the loop quantization: difference equations for wave functions on the space of triads need to be considered.

Such equations are often difficult to analyze or to solve explicitly (see [94, 95, 96, 97, 98] for some techniques), and especially difficult to interpret. Moreover, at such a fundamental level, the issue of how space-time emerges from the underlying quantum state becomes exceedingly difficult especially on inhomogeneous models with many degrees of freedom. This is an issue faced by any quantum theory of gravity, independently of the precise methods used. For a recent discussion in string theory, using the AdS/CFT correspondence, see [99]. Intuitive pictures then usually require the use of special models allowing exact solutions, which imposes more than just a class of symmetries such as also specific matter ingredients (a free, massless scalar, say). While such models can often be analyzed in great detail, their properties may or may not be typical for general cases even within the same class of symmetries. This is analogous to the classical situation where the simplest and best known cases of singularities (isotropic cosmology, Schwarzschild black hole) may not display the general behavior of classical singularities as they are shown to arise from singularity theorems are from more general studies. Nevertheless, since these types of singularities are quite relevant for our understanding of the universe, detailed pictures for how they can be resolved are valuable. Moreover, they can provide a basis for more general scenarios, for instance in a perturbation theory. The most common intuitive picture for such resolutions is a bounce.

6.1. Effective equations

Much intuition in cosmology derives from isotropic or at least homogeneous models where, from a semiclassical perspective, a bounce is the only way to resolve a classical singularity. There are only finitely many (at most three) metric components in those models which must stay away from zero to avoid a singularity. Thus, within a finite amount of time all components evolve through a minimum if they were initially contracting and thus lead to a bounce in volume. Note that this argument makes use of the finite dimensionality of the classical phase space and does thus not apply to inhomogeneous models. Moreover, the argument presupposes that some kind of semiclassical description at least of the quantum gravity state (if not matter fields) is valid throughout, which can then be identified with a smooth spatial geometry subject to an altered, bouncing dynamics.

While these assumptions are difficult to justify in general, or to be avoided in bounce arguments, bounce models can be useful to study semiclassical effects of quantum gravity. Moreover, if sufficiently well developed, they can be used to understand how cosmological inhomogeneities could evolve through a bounce with potential effects on structure formation. Rather surprisingly, one particular bounce model provides the zeroth order basis (“free theory”) for an effective theory of loop quantum gravity and a corresponding perturbation scheme. The technical details are fully analogous to the widely used low energy effective actions in particle physics and thus very promising for developing a detailed understanding of the semiclassical properties of loop quantum gravity.

6.1.1. Low energy effective action

It is often most useful to describe quantum effects in certain regimes by correction terms to classical equations, without changing the type of differential equations (except for possible higher derivative terms). Thus, a quantum mechanical system would still be formulated in terms of coupled ordinary differential equations in time rather than a

\[ \text{Some examples for bounces from loop effects can be found in [100, 101, 102, 103, 104, 74]}. \text{Oscillatory scenarios have been developed and described in [105, 106, 107, 108, 109].} \]
partial differential equation. Or, a quantum field theory would be described by partial differential equations in space-time coordinates rather than functional differential equations. This does not only lead to technical simplifications in solution procedures but also alleviates most interpretational issues of quantum theories.

In quantum mechanics, it is well-known that all harmonic oscillator states follow classical trajectories exactly. There is thus no need for modifications to classical equations of motion, and it turns out that only a zero point energy is added to the Hamiltonian \( H_Q = \frac{1}{2m} p^2 + \frac{1}{2} m \omega^2 q^2 + \frac{1}{2} \hbar \omega \). This is similar for free quantum field theories although the zero-point energy may diverge. For an-harmonic contributions \( U \) to the potential or for interactions, there are corrections to the classical Hamiltonian which can be computed in a perturbation theory around the harmonic oscillator or a free theory. By the usual particle physics techniques based on Legendre transforms of generating functionals of single wave packet) only in semiclassical regimes while they are defined here for an arbitrary quantum system. The justification for the term is that irrespective of the regime the quantum phase space is a fiber bundle over the classical phase space with bundle projection \( |\psi\rangle \rightarrow (\langle \psi|\hat{q}|\psi\rangle, \langle \psi|\hat{p}|\psi\rangle) \).

6.1.2. Quantum variables

A more useful set of coordinates for this purpose is defined as follows: we use “classical” variables:\[^1\]

\[
q = \langle \hat{q} \rangle \quad \text{and} \quad p = \langle \hat{p} \rangle
\]

\[^1\] This term often gives rise to confusion as these variables are close to the classical ones (e.g. in the sense of describing the peak position of a single wave packet) only in semiclassical regimes while they are defined here for an arbitrary quantum system. The justification for the term is that
and quantum variables

\[ G^{a,n} := \langle \{ \hat{q} - \langle \hat{q} \rangle \}^{n-a} (\hat{p} - \langle \hat{p} \rangle)^a \} \rangle_{\text{Weyl}} \]  

(33)

where \( n \geq 2, a = 0, \ldots, n \) and “Weyl” denotes the totally symmetric ordering of the operators before the expectation value is taken. Poisson relations of these variables are related to commutators as we will see in more detail later: \( \{ q, p \} = \{ [\hat{q}, \hat{p}] \} / \hbar = 1 \) and \( \{ q, G^{a,n} \} = 0 = \{ p, G^{a,n} \} \). For \( \{ G^{a,n}, G^{b,m} \} \) a closed formula exists but is rather lengthy [111] [112].

Quantum variables are dynamical just as the classical variables are: for a semiclassical state they change in time, e.g. if a wave packet spreads and deforms. The resulting evolution back-reacts on the classical variables which determine the peak position of the wave packet. Their motion then in general differs from the classical one, which is to be captured in appropriate quantum correction terms to the classical equations of motion. The exact behavior is determined by the Schrödinger equation, or equivalently by the quantum Hamiltonian \( H_Q \) which couples classical and quantum variables. For instance, for a cubic potential we have \( \langle \hat{q}^3 \rangle = q^3 + 6q^2 \hat{G}^{0,2} + 6 \hat{G}^{0,3} \) with a coupling term \( q \hat{G}^{0,2} \) in addition to a zero-point contribution by \( G^{0,3} \).

More generally, for an an-harmonic oscillator with classical Hamiltonian \( H = \frac{1}{2m} p^2 + \frac{1}{2} m \omega^2 q^2 + U(q) \) we have a quantum Hamiltonian with infinitely many coupling terms,

\[ H_Q = \langle H(\hat{q}, \hat{p}) \rangle = \langle H(q + \langle \hat{q} \rangle - q, p + \langle \hat{p} \rangle - p) \rangle \]

\[ = \frac{1}{2m} p^2 + \frac{1}{2} m \omega^2 q^2 + U(q) + \frac{\hbar \omega}{2} \hat{G}^{0,2} + \hat{G}^{2,2} + \sum_{n \geq 2} \frac{1}{n!} \left( \frac{\hbar}{m \omega} \right)^{n/2} U^{(n)}(q) \hat{G}^{0,n} \]  

(35)

written in dimensionless variables \( \hat{G}^{a,n} = \hbar^{-n/2}(m \omega)^{n/2-a} G^{a,n} \). As indicated, these terms follow from formally expanding the Hamiltonian in \( \hat{q} - q \) and \( \hat{p} - p \). Using the Poisson brackets of all classical and quantum variables, \( H_Q \) generates Hamiltonian equations of motion \( \hat{f} = \{ f, H_Q \} \):

\[ \dot{q} = \frac{p}{m} \]  

(36)

\[ \dot{p} = -m \omega^2 q - U'(q) - \sum_{n \geq 2} \frac{1}{n!} \left( \frac{\hbar}{m \omega} \right)^{n/2} U^{(n+1)}(q) \hat{G}^{0,n} \]  

(37)

\[ \dot{\hat{G}}^{a,n} = -a \omega \hat{G}^{a-1,n} + (n-a) \omega \hat{G}^{a+1,n} - a \frac{U''(q)}{m \omega} \hat{G}^{a-1,n} \]

\[ + \frac{\sqrt{\hbar} a U'''(q)}{2(m \omega)^{3/2}} G^{a-1,n-1} \hat{G}^{0,2} + \frac{\sqrt{\hbar} a U''''(q)}{3!(m \omega)^2} G^{a-1,n-1} \hat{G}^{0,3} \]

\[ - \frac{a}{2} \left( \frac{\sqrt{\hbar} U'''(q)}{(m \omega)^{3/2}} G^{a-1,n+1} + \frac{\sqrt{\hbar} U''''(q)}{3!(m \omega)^2} G^{a-1,n+2} + \ldots \right) \]  

(38)

These are infinitely many coupled equations for infinitely many variables. At this stage, the system is still fully equivalent to the Schrödinger dynamics, just written in terms of “n-point functions” \( q, p \) and \( G^{a,n} \) instead of the wave function they determine.

As an example we can look at the harmonic oscillator whose Hamiltonian equations of motion are

\[ \dot{p} = \{ p, H_Q \} = -m \omega^2 q \]

\[ \dot{q} = \{ q, H_Q \} = \frac{1}{m} p \]

\[ G^{a,n} = \{ G^{a,n}, H_Q \} = \frac{1}{m} (n-a) G^{a+1,n} - m \omega^2 a G^{a-1,n} \].

In this case, all terms coupling the \( G^{a,n} \) for different \( n \) vanish, and we have an infinite set of differential equations only finitely many of which are coupled to each other. Moreover, the equations are linear and can easily be solved. For instance, constant solutions for the quantum variables exist, satisfying uncertainty relations such as \( G^{0,2} G^{2,2} \geq \frac{\hbar^2}{4} + (G^{1,2})^2 \). These solutions correspond to the well-known coherent states which do not spread and follow the classical trajectories exactly. But even if quantum variables are not constant, they do not appear in equations of motion for the classical variables and thus do not back-react on them. This is why the effective action of the harmonic oscillator is identical to its classical action.
With an-harmonic contributions, coupling terms are switched on and all equations get coupled to each other. Consistent truncations to finitely many equations for finitely many variables are then required for an effective approximation. This is possible in, e.g., an adiabatic approximation [111]: we solve approximately for the leading \( G_{0,n} \) assuming that they change in time much more slowly than \( q \) and \( p \), and insert the solutions into the equations of motion for \( q \) and \( p \).

Doing this to first order in \( \hbar \) and to second order in the adiabatic approximation, and writing the first order equations for \( q \) and \( p \) as a second order equation for \( q \), we obtain

\[
\left( m + \frac{\hbar U''(q)^2}{32m^2 \omega^2 \left( 1 + \frac{U'(q)}{m \omega} \right)^{5/2}} \right) \ddot{q} + \frac{\hbar q}{128m^3 \omega^7} \left( 1 + \frac{U'(q)}{m \omega} \right)^{7/2} \frac{U'''(q)}{4m \omega \left( 1 + \frac{U'(q)}{m \omega} \right)^{1/2}} = 0
\]

as it also follows from the low energy effective action [30].

### 6.1.3. Solvable systems

The derivation clearly shows the role of the harmonic oscillator: its classical and quantum variables decouple to sets of finitely many linear equations and there is no back-reaction by quantum variables on expectation values. This happens whenever the Hamiltonian is quadratic in canonical variables, or more generally when the system is linear, i.e., when the Hamiltonian and a set of basic variables form a Lie algebra using Poisson brackets. Effective equations can then be obtained by perturbing around the exact solutions of such a solvable system.

Realizing this opens one possibility for generalizations of low energy effective equations, which are then based on alternative solvable systems suitable for a given context. Remarkably, examples for such solvable models are realized in cosmology and allow a systematic effective theory in this context.

### 6.2. Large scale effective theory for cosmological bounces

Identifying such a solvable model suitable for cosmology and deriving its perturbation equations allows one to derive intuitive semiclassical pictures which describe the transition through classical singularities in detail.

#### 6.2.1. Solvable model for cosmology

The harmonic oscillator with its periodic motion is not suitable as a solvable system for cosmology. But we can look at a free isotropic scalar model whose Friedmann equation \( c^2 \sqrt{\rho} = \frac{4 \pi G}{3} \rho - \frac{3}{2} \dot{p}_\phi^2 \) follows from (22) with variables \( c = \dot{a} \) (extrinsic curvature) and \( p^{3/2} = a^3 \) (volume) where \( \rho \) is the densitized triad component, now assumed positive. Solving for \( p_\phi \) yields \( p_\phi \propto c \rho =: H \), to be interpreted as the Hamiltonian which generates the flow in the variable \( \phi \) playing the role of internal time. This Hamiltonian is quadratic [112] although not of the harmonic oscillator form. But as in this case, classical and quantum variables decouple and the quantum Hamiltonian \( \hat{H} = \hat{c} \rho + \hat{G}^p \) is obtained, as in (35), by adding only the zero point contribution \( \hat{G}^p = \frac{1}{2} \left( \langle \hat{\dot{c}} \hat{\rho} \rangle + \langle \hat{\dot{\rho}} \hat{c} \rangle \right) - c \rho \). (Here, we use a slightly different notation compared to the general quantum variables [33] for better clarity.)

Its equations of motion follow by using Poisson brackets \( \{ c, G^p \} = 0 = \{ p, G^p \} \) as well as \( \{ G^c, G^p \} = 2G^c \), \( \{ G^G, G^P \} = 4G^P \), \( \{ G^G, G^{PP} \} = 2G^{PP} \) and further ones depending on which variables one is interested in solving.

---

12 We were not careful about the signs involved when solving the quadratic constraint equations for \( p_\phi \), although one can conclude from the constraint only that \( |p_\phi| \approx |c \rho| \). Using the absolute value for \( H \), on the other hand, would not leave it strictly quadratic. As we are mainly interested in states for which the expectation value of \( \hat{H} \) is large compared to the spread \( \Delta H \), we do not need to worry about significant contributions from solutions with different signs of the Hamiltonian. Note that \( H \) and \( \Delta H \) are preserved in time. Thus, if the condition \( H \gg \Delta H \) is satisfied once, e.g., for an initial semiclassical state, it will be satisfied at all values of \( \phi \).
for. We will now show how the relevant Poisson relations are derived, using the example of \( \{G^{0,2}, G^{1,2}\} \). The basic identity is the relation

\[
\{ \langle \hat{A}, \langle \hat{B} \rangle \} = \langle \hat{A}, [\hat{B}] \rangle / i\hbar
\]

(39)

which clearly shows how the quantum Poisson brackets are related to commutators. The familiar relation \( \{q, p\} = \langle \hat{q}, \hat{p} \rangle / i\hbar = 1 \) then follows immediately. But it cannot be directly applied to quantum variables such as \( G^{c} = \langle \hat{e}^{2} \rangle - c^{2} \) and \( G^{p} = \frac{1}{2}(\langle \hat{\dot{e}} \hat{p} \rangle + \langle \hat{\dot{p}} \hat{e} \rangle) - cp \) since here also products of expectation values occur. This can easily be dealt with using the Leibniz rule

\[
\{ f, g_{1} g_{2} \} = g_{1} \{ f, g_{2} \} + \{ f, g_{1} \} g_{2}
\]

(40)

to reduce all Poisson brackets to those of expectation values of operators where (39) applies. With the brackets \( \{ (\hat{e}^{2}), (\hat{\dot{e}} \hat{p}) \} = 2\langle e^{2} \rangle \), \( \{ (\hat{e}^{2}), (\hat{\dot{e}} \hat{p}) \} = \{ (\hat{\dot{e}}^{2}), (\hat{\dot{p}} \hat{e}) \} = 2\langle \dot{e}^{2} \rangle \) we then derive

\[
\{ G^{c}, G^{p} \} = \{ (\hat{e}^{2}) - c^{2}, \frac{1}{2}(\langle \hat{\dot{e}} \hat{p} \rangle + \langle \hat{\dot{p}} \hat{e} \rangle) - cp \} = 2\langle (\dot{e}^{2}) - c^{2} \rangle = 2G^{c}.
\]

Similarly, all other Poisson brackets are derived, for which also closed formulas exist [111, 112].

Equations of motion generated by \( H_{Q} = cp + G^{p} \) are thus \( \dot{c} = c, \dot{p} = -p \) for the classical variables, and \( G^{c} = 2G^{c}, G^{p} = 0 \) and \( G^{pp} = -2G^{pp} \) for the quantum variables. This is easily solved by \( c(t) = c_{1} e^{t}, p(t) = c_{2} e^{-t}, G^{c}(t) = c_{3} e^{2t}, G^{p}(t) = c_{4} \) and \( G^{pp}(t) = c_{5} e^{-2t} \) with suitable integration constants which are only restricted by the uncertainty relation \( c_{3} c_{5} \geq \hbar^{2}/4 + c_{4}^{2} \). Although constant solutions of the quantum variables do not exist, the semiclassical properties are quite similar to those of the harmonic oscillator. In particular, semiclassicality is preserved: the relative spreads are only exponentials \( \exp(\langle \hat{\dot{e}} \hat{p} \rangle / 2) \)

\[=\exp(\langle (\dot{e}^{2}) - c^{2} \rangle / 2)\]

which clearly shows how the quantum Poisson brackets are related to commutators. The familiar relation \( \{q, p\} = \langle \hat{q}, \hat{p} \rangle / i\hbar = 1 \) then follows immediately. But it cannot be directly applied to quantum variables such as \( G^{c} = \langle \hat{e}^{2} \rangle - c^{2} \) and \( G^{p} = \frac{1}{2}(\langle \hat{\dot{e}} \hat{p} \rangle + \langle \hat{\dot{p}} \hat{e} \rangle) - cp \) since here also products of expectation values occur. This can easily be dealt with using the Leibniz rule

\[
\{ f, g_{1} g_{2} \} = g_{1} \{ f, g_{2} \} + \{ f, g_{1} \} g_{2}
\]

(40)

to reduce all Poisson brackets to those of expectation values of operators where (39) applies. With the brackets

\[
\{ (\hat{e}^{2}), (\hat{\dot{e}} \hat{p}) \} = 2\langle e^{2} \rangle, \{ (\hat{\dot{e}}^{2}), (\hat{\dot{p}} \hat{e}) \} = \{ (\hat{\dot{e}}^{2}), (\hat{\dot{p}} \hat{e}) \} = 2\langle \dot{e}^{2} \rangle \text{ and } \{ c^{2}, cp \} = 2c^{2}
\]

we then derive

\[
\{ G^{c}, G^{p} \} = \{ (\hat{e}^{2}) - c^{2}, \frac{1}{2}(\langle \hat{\dot{e}} \hat{p} \rangle + \langle \hat{\dot{p}} \hat{e} \rangle) - cp \} = 2\langle (\dot{e}^{2}) - c^{2} \rangle = 2G^{c}.
\]

6.2.2. Loop formulation and bounces

In a loop formulation we do not use the Schrödinger quantization of basic variables \( c \) and \( p \). Instead, in a loop quantization [21] the operator \( \hat{p} \) has a discrete spectrum and no operator for \( c \) exists. What is represented are only exponentials \( \exp(ic) \) such that, e.g., \( \sin c \) occurs instead of \( c \). The resulting Hamiltonian operator \( \hat{H} = -\frac{1}{2}i(\exp(ic) - \exp(-ic))\hat{p} \) is a shift operator and implies a difference equation for the state in a triad representation. This operator is not identical to (23) derived earlier but is closely related. What we have not included here are quantum effects in the inverse power \( p^{-3/2} \) of the matter Hamiltonian as they occur in (25). Such terms do not allow solvable models but can be included in perturbation theory.

The Hamiltonian is non-quadratic and not solvable in an obvious way. But introducing \( \hat{J} = \hat{p}e^{ic} \) allows us to reorder the Hamiltonian to become a linear expression \( \hat{H} = -\frac{1}{2}i(\hat{J} - \hat{J}^{\dagger}) \). The price to pay is that the algebra of basic operators \( \hat{p} \) and \( \hat{J} \) is non-canonical, which usually implies that the system is not solvable in the above sense even for a linear Hamiltonian. But for the system under consideration it turns out that the set of Hamiltonian operator and basic variables \( \{\hat{p}, \hat{J} \} \) forms a linear system [113], given by the (trivially) centrally extended \( sl(2, \mathbb{R}) \) algebra

\[
\{ \hat{p}, \hat{J} \} = \hbar \hat{J} \quad , \quad \{ \hat{p}, \hat{J}^{\dagger} \} = -\hbar \hat{J}^{\dagger} \quad , \quad \{ \hat{J}, \hat{J}^{\dagger} \} = -2\hbar \hat{p} - \hbar^{2}.
\]

(41)

Taking expectation values, the linear quantum Hamiltonian \( H_{Q} = -\frac{1}{2}i(\hat{J} - \hat{J}^{\dagger}) \) does not even receive a zero point contribution and generates equations of motion

\[
p = \{ p, H_{Q} \} = -\frac{1}{2}(J + \bar{J}) \quad , \quad J = \{ J, H_{Q} \} = -\frac{1}{2}(p + \bar{h}) = \bar{J}
\]

(42)

with solution

\[
p(t) = \frac{1}{2}(c_{1} e^{-t} + c_{2} e^{t}) - \frac{1}{2}\bar{h} \quad , \quad J(t) = \frac{1}{2}(c_{1} e^{-t} - c_{2} e^{t}) + i\bar{h}.
\]

(43)

They are simply linear combinations of the solutions in the Schrödinger quantization. Depending on whether \( c_{1}c_{2} \) is positive or negative we have bouncing solutions of cosh form or solutions of sinh form which arrive at the classical singularity \( p = 0 \) after a finite amount of internal time \( t \). For our purpose of studying singularity removal we have to analyze these types of solutions in more detail.
FIGURE 16. Bouncing effective solutions for expectation value and spread.

But we have not yet implemented all necessary conditions and some of those solutions are non-physical. Classically we have \( J\bar{J} = p^2 \) for \( J = p \exp(ic) \), which as a reality condition for \( c \) must have an analog in the quantization. For states, this corresponds to normalizability in a physical inner product ensuring that \( \exp(ic) \) is quantized to a unitary operator. Although computing a physical inner product is usually a difficult issue, for the solutions \( p(t) \) and \( J(t) \) of expectation values we can implement the reality condition directly by just noticing that \( J\bar{J} = p^2 + O(\bar{\hbar}) \) must remain satisfied at the effective level. Only corrections of order \( \bar{\hbar} \) to the classical condition may result since \( \langle \hat{J} \hat{J}^\dagger \rangle \neq \langle \hat{J}^2 \rangle \).

The only way to implement this at all times is by requiring

\[
\frac{J\bar{J}}{(p + \bar{\hbar}/2)^2} = \frac{c_1 e^{-t} - c_2 e^t)^2 + 4H^2}{(c_1 e^{-t} + c_2 e^t)^2} = 1
\]

which implies \( c_1 c_2 = H^2 \) up to quantum corrections which are not important for large \( H \). This leaves only the bouncing solution

\[
p(t) = H \cosh(t - \delta) - \bar{\hbar}, \quad J(t) = -H(\sinh(t - \delta) + i)
\]

with a single constant of integration \( \delta \). Note that the minimum of \( p \) is given by \( H - \bar{\hbar} \) which for a large Hamiltonian \( H \), i.e. large matter content, is far away from the classical singularity at \( p = 0 \). The bounce trajectory agrees well with numerical solutions of (physically normalized) wave packets in a closely related model studied recently in [104, 114].

Similarly, we can compute equations of motion for the spread parameters

\[
G^{pp} = -2G^{pJ}, \quad G^{JJ} = 2G^{pJ}, \quad G^{pJ} = -\frac{1}{2}G^{JJ} - \frac{3}{4}G^{pp} - \frac{1}{2}(p^2 - JJ + \bar{\hbar}p + \bar{\hbar}^2/2)
\]

(46) (using \( \hat{J}\hat{J} = \hat{p}^2 \) and the commutation relations). They satisfy the uncertainty relation

\[
G^{pp}G^{JJ} - |G^{pJ}|^2 \geq \frac{\hbar^2}{4} |J|^2.
\]

For \( H \gg \hbar \), a solution is given by \( (\Delta p)^2 = G^{pp} \approx \hbar H \cosh(2(t - \delta_2)) \). The semiclassical behavior throughout the bounce is clearly seen from Fig. [16] where during the contraction and expansion phases the relative spreads are almost constant as in the Schrödinger quantization, although they may change from the contracting to the expanding phase depending on the integration constant \( \delta - \delta_2 \). The loop quantization thus connects the two branches in a well-defined way but leaves open the relative degrees of semiclassicaity on both sides.

6.2.3. Perturbations

As described in general terms before, perturbations around solvable models can be formulated by standard means. This allows one to introduce terms which imply couplings between classical and quantum variables, such as matter potentials, inhomogeneous degrees of freedom, or basic issues of a loop quantization. The latter effects include
different factor orderings of the constraint or modifications due to inverse powers in the matter Hamiltonian. This provides a systematic way to derive the evolution of fields through cosmological bounces, which is not available in other schemes where assumptions about the regularity at a bounce must be imposed rather than being derivable. The perturbation scheme mentioned here can certainly break down, which implies that the semiclassical nature of realistic bounces is testable in a self-consistent manner.

In addition to conceptual lessons, mechanisms for singularity resolution provide a possible relation to observations in bounce scenarios of structure formation, making use of Hamiltonian perturbation theory [115] and an implementation in perturbative loop quantum gravity [116].

7. THE CURRENT STATUS OF SINGULARITY RESOLUTION IN QUANTUM GRAVITY

We have focused the discussions here on the singularity problem from a general perspective. Accordingly, detailed scenarios we described were only those which have been formulated in a sufficiently general context, applying to more than a small class of situations and not showing any obvious limiting assumptions.

With recent developments, loop quantum cosmology has provided the first systematic effective theory for the non-singular evolution of perturbations through a classical singularity using perturbation theory around bouncing solutions. Expectation values and the spreading of semiclassical states can be computed explicitly. This shows under which circumstances semiclassical states are obtained also during and after the bounce, although the degree of semiclassicality depends on initial conditions. A general analysis is unfinished. In general, bounce pictures are difficult to extend to inhomogeneities unless the latter remain perturbative. Often, one appeals to the BKL conjecture to suggest that homogeneous scenarios might be sufficient to discuss singularity resolution. But by construction bounces in general do not allow one to go sufficiently deep in the regime, asymptotically close to a classical singularity, which is used in the BKL scenario to argue that time derivatives dominate spatial derivatives.

Under unrestricted perturbations, bounce pictures can easily break down and full quantum properties are required. Even in this case, singularity removal in loop quantum gravity is established in many situations by quantum hyperbolicity: wave functions on spaces of triads can be extended uniquely across classical singularities. This crucially rests on quantum geometry (rather than matter) and especially its discrete spatial structure. Background independence is important for the detailed realization, providing many consistency tests for quantum gravity. Quantum hyperbolicity is at present the most general mechanism for non-singular behavior, indeed showing clearly the role of important aspects of a background independent quantization of gravity. Nevertheless, much remains to be understood for a general statement on singularity resolution. The main problem at the current stage of developments is not only the complexity of quantum gravity, but also an understanding of the classical structure of singularities needed to select, in the absence of general solutions, the quantum regime to be looked at.

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