Quantum Cosmology

Claus Kiefer[1] and Barbara Sandhöfer[2]

[1] Institut für Theoretische Physik, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany. kiefer@thp.uni-koeln.de
[2] Institut für Theoretische Physik, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany. bs324@thp.uni-koeln.de

Summary. We give an introduction into quantum cosmology with emphasis on its conceptual parts. After a general motivation we review the formalism of canonical quantum gravity on which discussions of quantum cosmology are usually based. We then present the minisuperspace Wheeler–DeWitt equation and elaborate on the problem of time, the imposition of boundary conditions, the semiclassical approximation, the origin of irreversibility, and singularity avoidance. Restriction is made to quantum geometrodynamics; loop quantum gravity and string theory are discussed in other contributions to this volume.

To appear in *Beyond the Big Bang*, edited by R. Vaas (Springer, Berlin, 2008).

Denn wo keine Gestalt, da ist keine Ordnung; nichts kommt, nichts vergeht, und wo dies nicht geschieht, da sind überhaupt keine Tage, kein Wechsel von Zeiträumen.
Augustinus, Bekenntnisse, 12. Buch, 9. Kapitel

1 Why quantum cosmology?

Quantum cosmology is the application of quantum theory to the universe as a whole. At first glance, this may be a purely academic enterprise, since quantum theory is usually considered to be of relevance only in the micoroscopic regime. And what is more far remote from this regime than the whole universe? This argument is, however, misleading. In fact, quantum theory itself argues that the universe *must* be described in quantum terms. The reason is that every quantum system except the most microscopic ones are unavoidably and irreversibly coupled to their natural environment, that is, to a large number of degrees of freedom coupling to the system; an example would be a small dust grain in interaction with air molecules or photons. There exists then only one quantum state which *entangles* system and environment. The environment is itself coupled to its environment, and so on, leading ultimately to the whole universe as the only closed quantum system in the strict sense. It is entanglement with macroscopic degrees of freedom that also leads to the classical *appearance* of macroscopic bodies, a process known as decoherence. Decoherence is well understood theoretically and has been successfully tested in a variety of experiments [1]. The universe as a whole is thus at the same time of quantum nature and of classical appearance in most of its stages. There exist, of course, also situations where the latter does not hold and the quantum nature discloses itself; these are, in fact, the most interesting situations, some of which we shall discuss in the course of this article.

Conceptually, quantum cosmology is therefore not necessarily associated with quantum gravity. However, since gravity is the dominant interaction at large scales, any realistic framework of quantum cosmology must be based on a theory of quantum gravity. Although there is not yet an agreement on which is the correct theory, there exist various approaches such as quantum general relativity and string theory [2]. The purpose of the present article is to give a general introduction and some concrete models which are based on quantum geometrodynamics; we make only minor remarks on the more recent approach of loop quantum cosmology because this is covered in the contributions of Abhay Ashtekar and Martin Bojowald to this volume. Our emphasis is on the conceptual side; for more details we refer to [2] and the reviews [3, 4, 5, 6].

Quantum cosmology started in 1967 with Bryce DeWitt's pioneering paper [7]. He applied the quantization procedure to a closed Friedmann universe filled with matter. The latter is described phenomenologically, that is, not by a fundamental field. This is the first minisuperspace model of quantum cosmology. 'Minisuperspace' is the generic name for a cosmological model with only a finite number of degrees of freedom (such as the scale factor and an inflaton field). It originates from the fact that the full infinite-dimensional configuration space of general relativity is called 'superspace' and the prefix 'mini' is added for drastically truncated versions.

DeWitt already addressed some of the important issues in quantum cosmology, notably the singularity problem: can the singularity present in the classical theory be avoided in quantum cosmology? He suggested the boundary condition that the 'wave function of the universe' Ψ vanishes in the region where the classical singularity would appear, that is, at vanishing scale factor a. In fact, DeWitt advocates strongly the concept of a wave function of the universe and emphasizes the need to give up the 'Copenhagen' interpretation of quantum theory because no classical realm is a priori present in quantum cosmology.[3] This coincides with modern ideas in non-gravitational quantum

[3] To quote from [7]: "Everett's view of the world is a very natural one to adopt in the quantum theory of gravity, where one is accustomed to speak without embarassment of the 'wave function of the universe.' It is possible that Everett's view is not only natural but essential."

theory where classical properties are interpreted as emergent phenomena [1]. Incidentally, the linear structure of quantum theory remains untouched in almost all papers on quantum cosmology, so an Everett-type of interpretation is usually assumed, at least implicitly. DeWitt also addressed the important issue of the semiclassical approximation in quantum cosmology, on which we elaborate in Section 5 below.

Quantum cosmology was soon extended to anisotropic models, notably the Bianchi models, which are still homogeneous, but anisotropic and thus possess different scale factors for different spatial directions. Reviews of this early phase in quantum cosmology research include [8] and [9]. Minisuperspace models were usually used as illustrative examples to study conceptual issues in quantum gravity.

The second phase of quantum cosmology started in 1983 with the seminal paper by James Hartle and Stephen Hawking on the 'no-boundary proposal' [10]. This arose from a discussion of Euclidean path integrals in quantum gravity, which itself arose from black-hole thermodynamics. The idea is to sum in the path integral over Euclidean metrics that only possess one boundary (the present universe) and no other, 'initial', boundary. Other boundary conditions include the 'tunnelling condition', in which Ψ is supposed to contain only outgoing modes at singular boundaries of superspace [12] and the 'symmetric initial condition' [13]. The issue of boundary conditions is discussed in more detail in Section 4 below.

After the advent of the inflationary-universe scenario around 1980, it was also of interest to study the role of inflation in quantum cosmology. A particular issue was the question whether it makes sense to ask for the 'probability' of inflation and, if it does, to select the boundary condition from which inflation occurs most likely [2, 14]. Other issues concern the emergence of classical properties through decoherence, the arrow of time, and the origin of structure formation, some of which will be discussed below. Quantum cosmology was not only discussed for models arising from the quantization of general relativity, but also for more general situations such as string cosmology [15] or supersymmetry (SUSY) cosmology [16].

More recently, Martin Bojowald has introduced quantum cosmology into the framework of loop quantum gravity. A major new feature here is the occurrence of a difference (instead of a differential) equation for the wave function of the universe. This can lead to important results such as singularity avoidance and the presence of a repulsive contribution to the gravitational interaction that may be responsible for the occurrence of inflation. Loop quantum cosmology is discussed in the accompanying contribution by Ashtekar and Bojowald [17].

In the following, we shall first introduce the general framework of canonical quantum gravity and then apply it to quantum cosmology.

2 The formal framework: Quantum Gravity

There are several reasons why one should try to set up a quantum theory of gravity. The two main motivations come from quantum field theory and general relativity, respectively.

From a quantum field theoretical point of view, a unification of all fundamental interactions is an appealing aim. This would provide quantum field theory with a fundamental cut-off scale — not to mention the aesthetical aspect. Quantum gravity is then only one aspect of the ambitious venture to unify all interactions. The most prominent representative of such a theory is string theory.

From a general-relativistic perspective, a quantization of gravity is necessary to supersede general relativity. This is due to the remarkable fact that general relativity predicts its own break-down. This happens when quantities occuring in the theory itself diverge. The most famous example of such a divergence is the one ‘at’ the beginning of our Universe, coined the big-bang singularity.

In this context, quantum gravity stands for an effort to provide a quantum theory of the gravitational field. This can be done in more or less radical ways, depending on the amount of structure which one decides to keep classical and on the level at which one starts to quantize the theory’s elements. The most conservative approaches are content with a quantization of Einstein’s theory of general relativity. Such approaches are usually subdivided into *covariant* and *canonical* approaches: whereas the covariant approaches employ the covariance of spacetime at important parts of the formalism, the canonical approaches start with a split of spacetime into space and time and seek, in analogy to quantum mechanics, a Hamiltonian formalism in which the four-metric is interpreted as an evolution of a three-dimensional metric in time. Examples of covariant approaches are the path-integral approach and perturbation theory (derivation of Feynman diagrams); examples of canonical approaches are quantum geometrodynamics (the framework of this contribution) and loop quantum gravity.

The major alternative to the direct quantization of Einstein’s theory is string theory. The ambition of this theory is to provide a unified quantum theory of all interactions; quantum gravity is then only a particular aspect in a limit where gravity can be distinguished as a separate interaction. As for string-based quantum cosmology, we refer the reader to the corresponding contributions to this volume.

2.1 Canonical Quantum Gravity

(3 + 1)-Decomposition of General Relativity

At the basis of any canonical approach lies the Hamiltonian formulation of general relativity, cf. [2, 18]. To obtain such a formulation, one has to choose a foliation of spacetime; this is also called $(3+1)$-decomposition. Then one can define a Hamiltonian on each spatial hypersurface of this decomposition. General covariance is thus not explicit but recovered through the possibility to choose an arbitrary decomposition of four-dimensional spacetime into spatial hypersurfaces.[4] A scheme which provides us with just such a set-up is the so-called ADM-formulation of general relativity [19].

The peculiar feature of general relativity is that the Hamiltonian — usually decomposed into a part perpendicular and three components tangential to the spatial hypersurfaces — is constrained to vanish (We restrict ourselves to closed cosmologies; otherwise the Hamiltonian may contain boundary terms.). It is a linear combination of the four local constraints

$$\mathcal{H}_\perp(\mathbf{x}) = 0 \ , \qquad \mathcal{H}_a(\mathbf{x}) = 0 \ , \tag{1}$$

where $a = 1, 2, 3$. These constraints cover the entire dynamics of Einstein's theory and are equivalent to the Einstein equations. The occurrence of constraints is due to the fact that general relativity is a diffeomorphism-invariant theory (loosely speaking, this is the invariance under coordinate transformations). Figuratively speaking, diffeomorphism-invariance implies that spacetime points themselves cannot be endowed with any meaning in general relativity.

Canonical coordinates in this formalism are the three-dimensional metric, h_{ab}, on the spatial hypersurface and its conjugate momentum, related to the extrinsic curvature and denoted by p^{ab}. A different choice of canonically-conjugate coordinates is made in loop quantum gravity, cf. [2, 20] and the corresponding contributions to this volume. The $(3+1)$-decomposition is illustrated in Figures 1 (general case) and 2 (cosmological example).

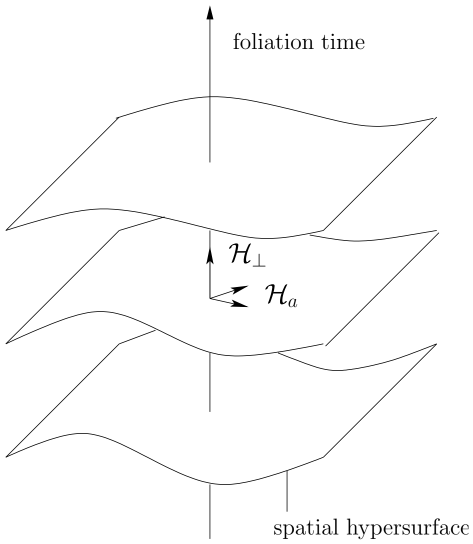
Quantization of the constraint system

Quantization can then be carried out in analogy to ordinary quantum theory: canonical coordinates are promoted to operators, thus turning the constraints into operators. These are implemented through the requirement

$$\widehat{\mathcal{H}}_\perp \Psi[h_{ab}] = 0 \ , \qquad \widehat{\mathcal{H}}_a \Psi[h_{ab}] = 0 \ , \tag{2}$$

where $\Psi[h_{ab}]$ is a wave functional depending on the three-metric. If non-gravitational fields are present, the wave functional depends in addition on them; for example, it may depend in addition on a scalar field ϕ. Here and in the following, operators will be denoted by hats on the corresponding quantities. The first equation is usually referred to as Wheeler–DeWitt equation.

[4] As an expression is independent of a choice of vector basis if no reference to that basis is made in the expression, independence of the choice of foliation is maintained if the choice of foliation does not occur in the final equations of the theory.



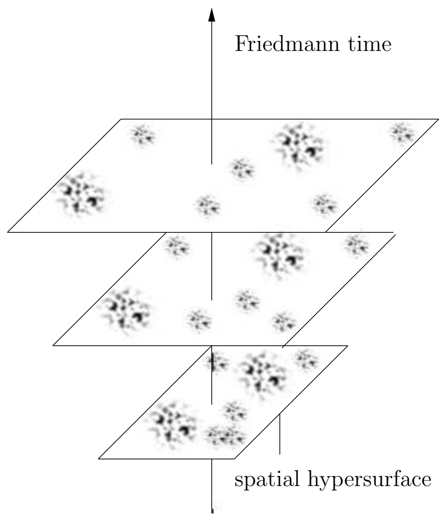


Fig. 1. The above plot shows the (3 + 1)-decomposition of a four-dimensional spacetime. Spatial hypersurfaces are stacked together along a foliation parameter. The components of the Hamiltonian tangential and perpendicular to the hypersurfaces are shown (but note that there are actually three components tangential to the hypersurfaces).

Fig. 2. Here, the decomposition is illustrated with the help of a cosmological example. The foliation is chosen such that spatial hypersurfaces are homogeneous and isotropic. On each such hypersurface we see galaxy clusters.

The other equations ensure invariance of the wave functional under three-dimensional diffeomorphisms. They are therefore known as diffeomorphism (or momentum) constraints.

In the classical theory, spacetime can be represented as a foliation of three-dimensional hypersurfaces. Since the canonical variables are the three-dimensional metric and the embedding of the hypersurfaces into the fourth dimension, both variables cannot be specified simultaneously in the quantum theory (they obey an 'uncertainty relation') – spacetime has disappeared. What remains is the configuration space which is the space of all three-geometries (called 'superspace' by John Wheeler).

What has been written down in a formal way here is in fact the origin of ambiguities in the set-up of a quantum theory of gravity. Promoting canonical coordinates to operators requires a choice of representation. And it is exactly at this point where the canonical path to quantum gravity branches out, yielding loop quantum gravity and quantum geometrodynamics as the most prominent directions. We will follow here the geometrodynamical path being given by the choice of Schrödinger representation of fundamental operators; for the alternative development which arises through a choice of the inequivalent loop representation, see the corresponding contributions to this volume. In geometrodynamics, then, the three-metric acts a multiplication operator and the momentum as a derivative operator,

$$\widehat{h}_{ab}\Psi[h_{ab}] = h_{ab}(\boldsymbol{x}) \cdot \Psi[h_{ab}] \;, \qquad \widehat{p}_{cd}\Psi[h_{ab}] = \frac{\hbar}{\mathrm{i}} \frac{\delta\Psi}{\delta h_{cd}(\boldsymbol{x})}[h_{ab}] \;, \tag{3}$$

where $\mathbf{x}$ denotes a point in the hypersurface. With this choice of representation, the governing quantum equations read

$$\left(-16\pi G\hbar^2 G_{abcd} \frac{\delta^2}{\delta h_{ab}\delta h_{cd}} - \frac{\sqrt{h}}{16\pi G}({}^{(3)}R - 2\Lambda) \right) \Psi = 0 \;, \tag{4}$$

$$-2D_b h_{ac} \frac{\hbar}{\mathrm{i}} \frac{\delta\Psi}{\delta h_{bc}} = 0 \;. \tag{5}$$

These equations are of a formal nature, since the factor-ordering problem and the regularization issue have not been addressed. Here, G is the gravitational constant and $\hbar$ Planck's constant, i is the imaginary unit.[5] The first, Wheeler–DeWitt, equation contains two terms. The first term with the structure of a kinetic energy term contains second derivatives with respect to the metric on spatial hypersurfaces, h_{ab}. They are connected through the so-called DeWitt metric G_{abcd}. The second term, acting as a potential, enters with a factor containing the square root of the determinant of the three-metric, h. It has two contributions, one coming from the three-dimensional Ricci scalar ${}^{(3)}R$ and, counteracting this, the cosmological constant Λ. The diffeomorphism constraint equations contain a covariant derivative D_b of the 3-metric. The equation is of a similar form as the Gauss constraint in quantum electrodynamics. If, in addition to the gravitational field, matter fields are present, the equations are augmented by the corresponding terms [2]. Even though most conceptual features of this set of constraint equations can be discussed at the fundamental level, we will now turn to cosmological examples to illustrate them.

3 Wheeler–DeWitt equation

In homogeneous cosmologies, the diffeomorphism constraint is satisfied trivially. What remains is the Wheeler–DeWitt equation, which is at the heart of

[5] The speed of light is set equal to one. It can be restored by the substitution $G \to G/c^4$.

any canonical approach to quantum cosmology, independent of the choice of representation.[6] It is the analogue of the (functional) Schrödinger equation in quantum field theory.[7]

To be more precise, consider the simplest setting, a homogeneous, isotropic Friedmann cosmology filled with a perfect cosmological fluid. This is an example of a 'minisuperspace model'. As we are aiming at a quantum theory, instead of an effective description of the cosmological fluid in terms of its energy density and pressure, we use a fundamental Lagrangian, namely that of a scalar field. The scalar field thus serves as a surrogate for the matter content of the universe. Our fundamental equation is then given by (see the Appendix for a derivation)

$$\begin{aligned}\hat{\mathcal{H}}\Psi = \Bigg(& \frac{2\pi G\hbar^2}{3}\frac{\partial^2}{\partial\alpha^2} - \frac{\hbar^2}{2}\frac{\partial^2}{\partial\phi^2} \\ & + e^{6\alpha}\left(V(\phi) + \frac{\Lambda}{8\pi G}\right) - 3e^{4\alpha}\frac{k}{8\pi G}\Bigg)\Psi(\alpha,\phi) = 0\ ,\end{aligned} \tag{6}$$

with cosmological constant Λ and curvature index $k = \pm 1, 0$. The variable $\alpha = \ln a$, where a stands for the scale factor, is introduced to obtain a convenient form of the equation.

As it stands, this is actually an understatement of the importance of this step. The introduction of the variable α is necessary to endow the Wheeler–DeWitt equation with a quantity which ranges from negative to positive infinity. Indeed the rôle of the variable α is two-fold: it leaves us with positive values for the scale factor *and* makes the Wheeler–DeWitt equation well-defined at the big bang. This can be seen from the original form of the Wheeler–DeWitt equation containing a,

$$\begin{aligned}\hat{\mathcal{H}}\Psi = \Bigg(& \frac{2\pi G\hbar^2}{3a^2}\frac{\partial}{\partial a}\left(a\frac{\partial}{\partial a}\right) - \frac{\hbar^2}{2a^3}\frac{\partial^2}{\partial\phi^2} \\ & + a^3\left(V(\phi) + \frac{\Lambda}{8\pi G}\right) - 3a\frac{k}{8\pi G}\Bigg)\Psi(a,\phi) = 0\ .\end{aligned} \tag{7}$$

This equation obviously contains terms that diverge as the big bang (or the big crunch) is approached, $a \to 0$. Through a transformation on α we obtain (6) multiplied by an overall factor of $e^{-3\alpha}$. But this factor is non-zero and can be removed, leaving the well-defined equation (6).[8]

---

[6] In loop quantum cosmology it takes the form of a difference equation.

[7] Rumour has it that DeWitt tried to establish the name 'Einstein–Schrödinger equation' for this equation. However, these efforts were to no avail [20, 7].

[8] The attempts to implement the positivity of the metric into the fundamental commutation relations leads to the approach of 'affine quantum gravity' [21]. As far as quantum cosmology is concerned, this approach is very close to the approach presented here.

Quantization of the Hamiltonian constraint thus provides quantum cosmology with a central equation of equal importance as the Schrödinger equation in quantum mechanics. But there are some obvious differences to the Schrödinger equation which cannot go without comment and which will be discussed in the following subsections.

3.1 An equation in configuration space

Most obviously, the Wheeler–DeWitt equation is a partial differential equation determining a wave function which is *not* defined in space or time or spacetime. It is an equation defined in configuration space, that is, it depends on the gravitational and matter degrees of freedom of the system (in this example α and ϕ) — not on spacetime points. This is in fact what one would expect from the quantization of a diffeomorphism-invariant theory such as general relativity. In general relativity, a spacetime point has no physical significance. It can be assigned significance only through a physical field. That is why we find not points but fields as the arguments of the wave function.

3.2 A timeless equation

Furthermore, this equation lacks an external time parameter. If we think of the Wheeler–DeWitt equation as the analogue of the Schrödinger equation, the most striking difference is the lack of a first derivative with an imaginary factor. This is what, in quantum mechanics, distinguishes space from time: time t is represented by a real number, and the positions are represented by operators. In special relativistic quantum field theory, spacetime plays the role of the external time, and the dynamical quantum fields are represented by operators. In quantum gravity, spacetime has disappeared and only the quantum fields (defined on space) remain.

Apart from the observation that we have no coordinate and thus also no time-coordinate dependence in the Wheeler–DeWitt equation, we find that we have no preferred evolution parameter. This is usually called the *problem of time*: the absence of an external time parameter and the non-uniqueness of internal timelike variables. This fact has caused much confusion at the advent of canonical quantum gravity. There are basically two types of reaction to this observation.

Time before quantization — internal time

One possibility to cope with this situation is to try to recover the form of the Schrödinger equation in some way. The basic idea is to rewrite the classical constraints in such a way that upon quantization, a Schrödinger-type equation is obtained. On the classical level, the rewritten constraints thus have to be of the form

$$\mathcal{P}_A + h_A = 0 \ , \tag{8}$$

that is, one needs a linear canonical momentum $\mathcal{P}_A$ for which one can solve the constraint; h_A simply stands for the remaining terms. Upon quantization one obtains

$$\mathrm{i}\hbar \frac{\delta \Psi}{\delta q_A} = \widehat{h}_A \Psi \ , \tag{9}$$

which is a Schrödinger-type equation It is in general inequivalent to the Wheeler–DeWitt equation. Usually, h_A is referred to as 'physical Hamiltonian' because it actually describes an evolution in a *physical* parameter, namely the coordinate q_A conjugate to $\mathcal{P}_A$. Time, in the sense of a physical evolution parameter, is therefore defined *before* quantization. As a result, time is part of an a priori background structure.

Primary research in this direction tried to actually solve the constraints of general relativity, separating the true, dynamical from the gauge degrees of freedom. This attempt to cope with the timelessness of quantum gravity suffers from several conceptual as well as technical difficulties; for a full list see [22, 23, 2]. An example of a conceptual problem is the fact that the choice of time variable is not unique. It is not clear what conditions a variable has to satisfy in order to qualify as an internal time. Neither is it clear that, could such conditions be specified, they would leave a unique choice of time.

In the simple cosmological case, one could, for example, choose the scale factor but equally well the scalar field ϕ as internal time. But one could as well choose one of the canonical momenta, for example the one related to the scale factor, π_a, as internal time coordinate. From these choices result non-unitary, that is, inequivalent, quantum theories. It is unclear how predictions resulting from different such choices are related (if they are related at all).

Technically, the heaviest blow came from a result by Charles Torre who proved that a global solution to the constraints does not exist in general relativity [24]. In consequence, advocates of this interpretation of the constraint equations turned to 'matter clocks' [23]. A matter clock is a type of matter whose Hamiltonian is of such a form that the full Hamiltonian is again of the form (8); that is, the matter Hamiltonian has to be linear in momentum and describe physical clocks (e. g. they should run forward). This was already a last-ditch effort. It lost its followers when it became clear that one either had to choose a Hamiltonian which described a physical clock but no physical matter or vice versa.

The reason why the internal time idea is nevertheless discussed here is that it was recently revived in the context of loop quantum cosmology. So far, cosmological models studied in this area use a Schrödinger-type equation describing evolution in an (often massless) scalar field. Apart from the choice of fundamental variables and the choice of representation of operators, this is another difference separating loop quantum cosmology from quantum geometrodynamical cosmological research.

Time after quantization — the frozen formalism

An opposite strategy is to identify time *after* quantization. Here, the Wheeler–DeWitt equation is taken at face value and no rewriting on the classical level is made before quantization. The crucial observation here goes back to DeWitt who accentuated the hyperbolic form of the Wheeler–DeWitt equation [7].[9] The hyperbolic form distinguishes a particular part of the gravitational degree of freedom (its conformal part, which in the above model is just the scale factor a) from the remaining degrees of freedom: its second-derivative term has a positive prefactor, whereas the derivatives with respect to the remaining degrees of freedom enter with a minus sign. In this spirit, it seems sensible to impose boundary conditions for fixed gravitational degree of freedom, $a =$ constant.

Problems of this point of view are all related to the lack of time structure. There seems to be no way to define a positive definite inner product in general models. Thus we have no handle on the interpretation of the wave function. Related to this is the question whether operators, for example, the constraint operators, should be self-adjoint. But all these problems which at the dawn of quantum gravity drove researchers to the internal-time idea, are due to the fact that we have no a priori notion of time. As our understanding of quantum gravity has improved, we may be able to challenge our brain with this further loss of structure. Inner products and self-adjoint operators are then reserved for a semi-classical world where a notion of time can be recovered, see Section 5. In the following we will adopt this point of view.

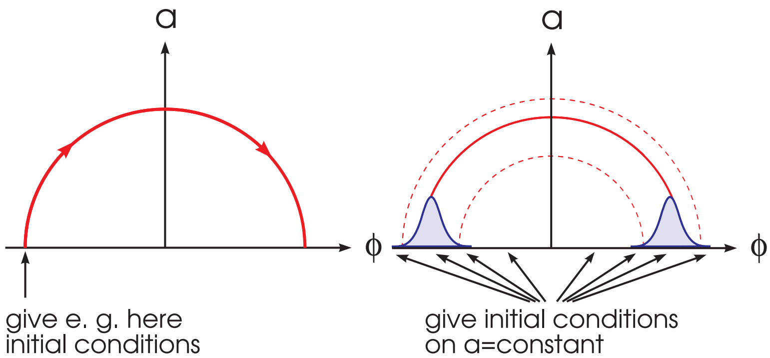
3.3 Determinism of wave packets

The two rather straight observations made above concerning the structure of the Wheeler–DeWitt equation converge to produce a peculiar notion of determinism on the level of quantum cosmology. Despite the absence of an *external* time parameter, the equation is of hyperbolic form thus suggesting to use the 3-volume v or $\alpha = \frac{1}{3}\ln v$ as an *intrinsic* time parameter [26]. The term 'intrinsic time parameter' denotes an evolution parameter of the equation, generally unrelated to any physical notion of time (which on the quantum level is anyway lost, as discussed above). Exchanging the classical differential equations in time for a timeless differential equation hyperbolic in α alters the determinism of the theory. This, of course, changes the way in which boundary conditions can be imposed. Wave packets are not evolved with respect to Friedmann time but with respect to intrinsic time. This turns our notion of determinism on the head.

[9] Thus, in structure, the Wheeler–DeWitt equation resembles the Klein–Gordon equation rather than the Schrödinger equation. Consequently, it suffers from the same problems as the former one (lack of positive-definiteness of the inner product).

This is illustrated by the following example. Simplify the universe model with the two degrees of freedom a (scale factor) and ϕ (scalar field) underlying (7) by the assumption $\Lambda = 0$. Take, moreover, the scalar field to be massless and the universe to be closed, $k = 1$. This model has a classical solution evolving from big bang to big crunch. The trajectories in configuration space are depicted in Figure 3 where the arrow along the trajectory signifies increasing Friedmann time.

Fig. 3. The classical and the quantum theory of gravity exhibit drastically different notions of determinism. The scalar field ϕ is shown on the horizontal axis, while the scale factor a of the universe is shown on the vertical axis.



Classically, one imposes initial conditions at $t = t_0$, corresponding to the left intersection of the trajectory with the ϕ-axis. These initial conditions determine the evolution of a and ϕ into the big-crunch singularity. Not so in quantum cosmology. Here, initial conditions have to be imposed at $a = 0$. If the wave packet shall follow the classical trajectory, one has to impose two wave packets at each intersection point of the classical trajectory with the $a = 0$ line. Wave packets are evolved from both, classical big-bang and big-crunch singularity, in the direction of increasing a; big bang and big crunch are intrinsically indistinguishable.[10]

[10] One should remark that the hyperbolicity with respect to the three-volume is an inherent feature of the Wheeler–DeWitt equation only as long as we are working in physically conventional settings. A counter-example is given by a non-minimally coupled scalar field. In this case, regions in configuration space exist in cosmological models where the quantum equation becomes elliptic [27]. Moreover, implementation of more exotic types of matter may also destroy the hyperbolicity of the Wheeler–DeWitt equation. Including, for example, a phantom field mimicked by a homogeneous scalar field with reversed sign of the kinetic energy term, yields an ultrahyperbolic equation [28]. An evolution of initially imposed wave packets at $a =$ constant is not justified in these cases by the form of the Wheeler–DeWitt equation.

4 Boundary Conditions

As we have discussed above, implementing boundary conditions in quantum cosmology differs from the situation in both general relativity and ordinary quantum mechanics. In the following we shall briefly review two of the most widely discussed boundary conditions: the 'no-boundary proposal' and the 'tunnelling proposal'. More details can be found in [2].

4.1 No-boundary proposal

Also called the 'Hartle–Hawking proposal' [10], the no-boundary proposal is basically of a topological nature. It is based on the Euclidean path integral representation for the wave function,

$$\Psi[h_{ab}] = \int \mathcal{D}g_{\mu\nu}(x)\, \mathrm{e}^{-S[g_{\mu\nu}(x)]/\hbar} \ , \tag{10}$$

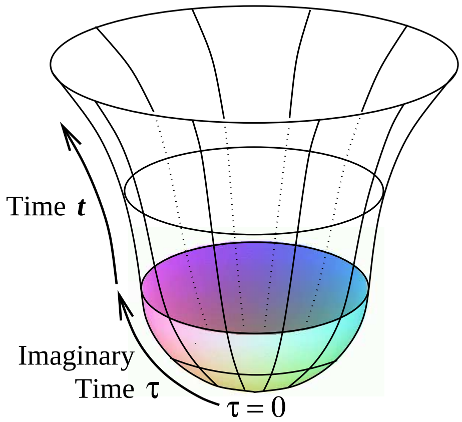
in which S is the classical action of general relativity and $\mathcal{D}g_{\mu\nu}(x)$ stands for the integration measure - a sum over all four-geometries. (In general, one also sums over matter fields.) 'Euclidean' means that the time variable is assumed to be imaginary ('imaginary time').

Since the full path integral cannot be evaluated exactly, one usually resorts to a saddle-point approximation in which only the dominating classical solutions are taken into account to evaluate S. The proposal, then, consists of two parts. First, it is assumed that the Euclidean form of the path integral is fundamental, and that the Lorentzian structure of the world only emerges in situations where the saddle point is complex. Second, it is assumed that one integrates over metrics with one boundary only (the boundary corresponding to the present universe), so that no 'initial' boundary is present; this is the origin of the term 'no-boundary proposal'. The absence of an initial boundary is implemented through appropriate regularity conditions. In the simplest situation, one finds the dominating geometry depicted in Figure 4, which is often called the 'Hartle–Hawking instanton', but which was already introduced by Vilenkin [11]: the dominating contribution at small radii is (half of the) Euclidean four-sphere S^4, whereas for bigger radii it is (part of) de Sitter space, which is the analytic continuation of S^4. Both geometries are matched at a three-geometry with vanishing extrinsic curvature. The Lorentzian nature of our universe would thus only be an 'emergent' phenomenon: standard time t emerges only during the 'transition' from the Euclidean regime (with its imaginary time) to the Lorentzian regime.

From the no-boundary proposal one can find for the above model with the massive scalar field (and vanishing Λ) the following wave function in the Lorentzian regime:

$$\psi_{\mathrm{NB}} \propto \left(a^2V(\phi)-1\right)^{-1/4} \exp\left(\frac{1}{3V(\phi)}\right) \cos\left(\frac{(a^2V(\phi)-1)^{3/2}}{3V(\phi)} - \frac{\pi}{4}\right) \ . \tag{11}$$

Fig. 4. 'Hartle–Hawking instanton': the dominating contribution to the Euclidean path integral is assumed to be half of a four-sphere attached to a part of de Sitter space. Obviously, this is a singularity-free four-geometry. This instanton demonstrates clearly the no-boundary proposal in that there is no boundary at $\tau = 0$.



In more general situations, one has to look for integration contours in the space of complex metrics that render the integral convergent. In concrete models, one can then find a class of wave functions which is a subclass of the solutions to the Wheeler–DeWitt equation. In this sense, the boundary condition picks out particular solutions. Unfortunately, the original hope that only one definite solution remains, cannot be fulfilled.

4.2 Tunnelling proposal

The tunnelling proposal emerged from the work by Alexander Vilenkin, cf. [11, 12] and references therein. It is most easily formulated in minisuperspace. In analogy with, for example, the process of α-decay in quantum mechanics, it is proposed that the wave function consists solely of *outgoing* modes. More generally, it states that it consists solely of outgoing modes at singular boundaries of superspace (except the boundaries corresponding to vanishing three-geometry). In the minisuperspace example above, this is the region of infinite a or ϕ. What does 'outgoing' mean? The answer is clear in quantum mechanics, since there one has a reference phase $\propto \exp(-\mathrm{i}\omega t)$. An outgoing plane wave would then have a wave function $\propto \exp(\mathrm{i}kx)$. But since there is no external time t in quantum cosmology, one has to *define* what 'outgoing' actually shall mean [26, 29]. Independent of this reservation, the tunnelling proposal picks out particular solutions from the Wheeler–DeWitt equation. The interesting fact is that these solutions usually differ from the solutions picked out by the no-boundary proposal: whereas the latter yields real solutions, the solutions from the tunnelling proposal are complex; the real exponential prefactor differs in the sign of the exponent. Explicitly, one gets in the above model the following wave function:

$$\psi_{\mathrm{T}} \propto (a^2V(\phi)-1)^{-1/4}\exp\left(-\frac{1}{3V(\phi)}\right)\exp\left(-\frac{\mathrm{i}}{3V(\phi)}(a^2V(\phi)-1)^{3/2}\right) . \tag{12}$$

Comparing this with (11), one recognizes that the tunnelling proposal leads to a wave function different from the no-boundary condition. Consequences of this difference arise, for example, if one asks for the probability of an inflationary phase to occur in the early universe: whereas the tunnelling proposal seems to favour the occurrence of such a phase, the no-boundary proposal seems to disfavour it. No final word on this issue has, however, been spoken.

5 Inclusion of inhomogeneities and the semiclassical picture

Realistic models require the inclusion of further degrees of freedom; after all, our Universe is not homogeneous. This is usually done by adding a large number of multipoles describing density perturbations and small gravitational waves [32, 2]. One can then derive an approximate Schrödinger equation for these multipoles, in which the time parameter t is defined through the minisuperspace variables (for example, a and ϕ). The derivation is performed by a Born–Oppenheimer type of approximation scheme. The result is that the total state (a solution of the Wheeler–DeWitt equation) is of the form

$$\Psi \approx \exp(\mathrm{i}S_0[h_{ab}]/\hbar)\,\psi[h_{ab},\{x_n\}] \ , \tag{13}$$

where h_{ab} is here again the three-metric, S_0 is a function of the three-metric only, and $\{x_n\}$ stands for the inhomogeneities ('multipoles'). In short, one has that

- S_0 obeys the Hamilton–Jacobi equation for the gravitational field and thereby defines a classical spacetime which is a solution to Einstein's equations (this order is formally similar to the recovery of geometrical optics from wave optics via the eikonal equation).
- ψ obeys an approximate Schrödinger equation,

$$\mathrm{i}\hbar\underbrace{\nabla S_0\,\nabla\psi}_{\equiv\frac{\partial\psi}{\partial t}} \approx H_{\mathrm{m}}\,\psi \ , \tag{14}$$

  where H_{m} denotes the Hamiltonian for the multipole degrees of freedom. The ∇-operator on the left-hand side of (14) is a shorthand notation for derivatives with respect to the minisuperspace variables (here: a and ϕ). Semiclassical time t is thus defined in this limit from dynamical variables, and is *not* prescribed from the outside.

- The next order of the Born-Oppenheimer scheme yields quantum gravitational correction terms proportional to G [30, 2]. The presence of such terms may in principle lead to observable effects, for example, in the anisotropy spectrum of the cosmic microwave background radiation.

The Born–Oppenheimer expansion scheme distinguishes a state of the form (13) from its complex conjugate. In fact, in a generic situation where the total state is real, being for example a superposition of (13) with its complex conjugate, both states will decohere from each other, that is, they will become dynamically independent [1]. This is a type of symmetry breaking, in analogy to the occurrence of parity violating states in chiral molecules. It is through this mechanism that the i in the Schrödinger equation emerges. Quite generally one can show how a classical geometry emerges from quantum gravity in the sense of decoherence [1]: irrelevant degrees of freedom (such as density perturbations or small gravitational waves) interact with the relevant ones (such as the scale factor or the relevant part of the density perturbations), which leads to quantum entanglement. Integrating out the irrelevant variables (which are contained in the above multipoles $\{x_n\}$) produces a density matrix for the relevant variables, in which non-diagonal (interference) terms become small. One can show that the universe assumes classical properties at the onset of inflation [1, 2].

The recovery of the Schrödinger equation (14) raises an interesting issue. It is well known that the notion of Hilbert space is connected with the conservation of probability (unitarity) and thus with the presence of an external time (with respect to which the probability is conserved). The question then arises whether the concept of a Hilbert space is still required in the *full* theory where no external time is present. It could be that this concept makes sense only on the semiclassical level where (14) holds, cf. our remarks at the end of Section 3.2.

Of course, the last word on quantum cosmology has not been spoken as long as we have no consensus on the interpretation of the wave function. What makes this issue so troublesome, is the missing link of a wave function of the universe to measurement. The measurement process supplies quantum mechanics with a probability interpretation. The potentiality of measurement yields sense to the Hilbert space structure. Expectation values are interpreted as possible outcomes of measurements with probability depending on the state the measured system is in. This interpretation entails the normalizability requirement for the wave function. Moreover, probabilities have to be conserved in time.

The problem is that we have no measurement crutch in quantum cosmology. This is a problem that persists also in the full theory and is a consequence of background independence. Only in a background of space and time can we make observations. An expectation value formulated in a theory deprived of that background is deprived of its interpretation (and justification) through measurement.

A background independent quantum theory may thus be freed from a physical Hilbert space structure.[11] It should keep linearity, since the superposition principle is not linked to observation, but it should dismiss the inner product as it is not clear how to endow it with a meaning in a timeless context (a clear statement on these issues is given in [33]). A Hilbert-space structure may, however, be needed on an effective level for quantum gravitational systems embedded in a semiclassical universe; a typical situation is a quantum black hole [31]. Due to the linear structure of quantum gravity, the total quantum state is a superposition of many macroscopic branches even in the semiclassical situation, each branch containing a corresponding version of the observer (the various versions of the observer usually do not know of each other due to decoherence). This is often referred to as the 'many-worlds (or Everett) interpretation of quantum theory', although only one *quantum* world (described by the full Ψ) exists.

We saw here that classical structures such as time arise only under certain conditions. It is in these regimes that we expect a physical Hilbert-space structure. Only here can we make connnection with measurements.

6 Arrow of time and structure formation

Although most fundamental laws are invariant under time reversal, there are several classes of phenomena in Nature that exhibit an arrow of time [34]. It is generally expected that there is an underlying master arrow of time behind these phenomena, and that this master arrow can be found in cosmology. If there existed a special initial condition of low entropy, statistical arguments could be invoked to demonstrate that the entropy of the universe will increase with increasing size.

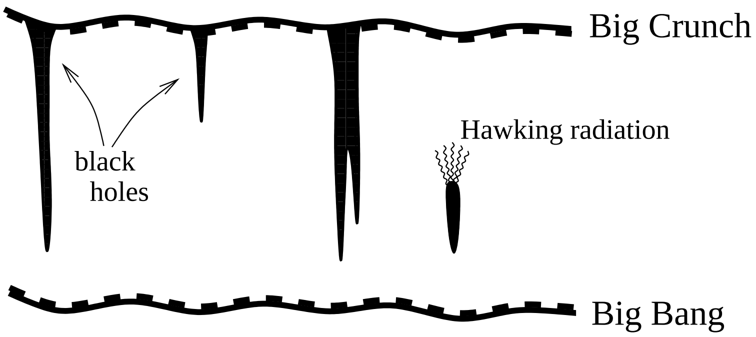
There are several subtle issues connected with this problem. First, one does not yet know a general expression for the entropy of the gravitational field; the only exception is the black-hole entropy, which is given by the expression

$$S_{\rm BH} = \frac{k_{\rm B} c^3 A}{4G\hbar} = k_{\rm B} \frac{A}{4l_{\rm P}^2} \ , \tag{15}$$

where A is the surface area of the event horizon, $l_{\rm P}$ is the Planck length and $k_{\rm B}$ denotes Boltzmann's constant. According to this formula, the most likely state for our universe would result if all matter would assemble into a gigantic black hole; this would maximize (15). More generally, Roger Penrose has suggested to use the Weyl tensor as a measure of gravitational entropy [34]. The cosmological situation is depicted in Figure 5 which expresses the very special nature of the big bang (small Weyl tensor) and the generic nature of a big crunch (large Weyl tensor). Entropy would thus increase from big bang to big crunch.

[11] This does not pertain the necessity to define an auxiliary or kinematical Hilbert space in order to define (not necessarily self-adjoint) operators.

Fig. 5. The classical situation for a recollapsing universe: the big crunch is fundamentally different from the big bang because the big bang is very smooth (low entropy), whereras the big crunch is very inhomogeneous (high entropy). Adapted from [34].



Second, since these boundary conditions apply in the very early (or very late) universe, the problem has to be treated within quantum gravity. But as we have seen, there is no external time in quantum gravity – so what does the notion 'arrow of time' mean?

We shall address this issue in quantum geometrodynamics, but the situation should not be very different in loop quantum cosmology or string cosmology. An important observation is that the Wheeler–DeWitt equation exhibits a fundamental asymmetry with respect to the 'intrinsic time' defined by the sign of the kinetic term. Very schematically, one can write this equation as

$$H\Psi = \left(\frac{\partial^2}{\partial\alpha^2} + \sum_i \left[-\frac{\partial^2}{\partial x_i^2} + \underbrace{V_i(\alpha, x_i)}_{\to 0 \text{ for } \alpha\to-\infty} \right] \right) \Psi = 0 \ , \tag{16}$$

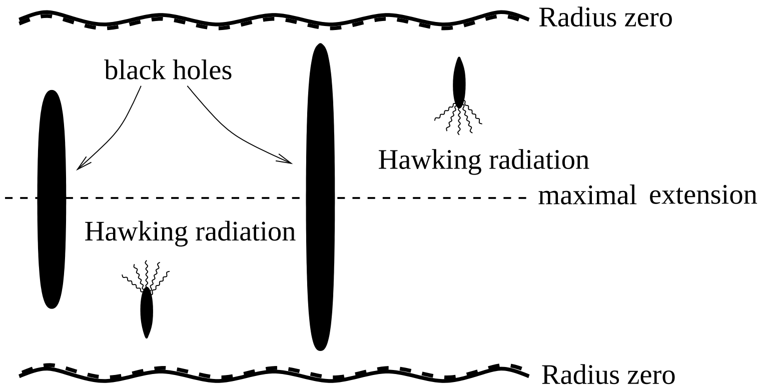
where again $\alpha = \ln a$, and the $\{x_i\}$ again denote inhomogeneous degrees of freedom describing perturbations of the Friedmann universe (see above); $V_i(\alpha, x_i)$ are the potentials of the inhomogeneities. The important property of the equation is that the potential becomes small for $\alpha \to -\infty$ (where the classical singularities would occur), but complicated for increasing α; the Wheeler–DeWitt equation thus possesses an asymmetry with respect to 'intrinsic time' α. One can in particular impose the simple boundary condition

$$\Psi \quad \stackrel{\alpha\to-\infty}{\longrightarrow} \quad \prod_i \psi_i(x_i) \ , \tag{17}$$

which would mean that the degrees of freedom are initially *not* entangled. Defining an entropy as the entanglement entropy between relevant degrees of freedom (such as α) and irrelevant degrees of freedom (such as most of the

$\{x_i\}$), this entropy vanishes initially but increases with increasing α because entanglement increases due to the presence of the potential. In the semiclassical limit where t is constructed from α (and other degrees of freedom), cf. (14), entropy increases with increasing t. This then *defines* the direction of time and would be the origin of the observed irreversibility in the world. The expansion of the universe would then be a tautology. Due to the increasing entanglement, the universe rapidly assumes classical properties for the relevant degrees of freedom due to decoherence [1, 2]. Decoherence is here calculated by integrating out the $\{x_i\}$ in order to arrive at a reduced density matrix for α.

Fig. 6. The quantum situation for a 'recollapsing universe': big crunch and big bang correspond to the same region in configuration space. Adapted from [34].



This process has interesting consequences for a classically recollapsing universe [35, 34]. Since big bang and big crunch correspond to the same region in configuration space ($\alpha \to -\infty$), an initial condition for $\alpha \to -\infty$ would encompass both regions, cf. Figure 3. This would mean that the above initial condition would always correlate increasing size of the universe with increasing entropy: the arrow of time would formally reverse at the classical turning point. big bang and big crunch would be identical regions in configuration space. The resulting time symmetric picture is depicted in Figure 6, which has to be contrasted with Figure 5. As it turns out, however, a reversal cannot be observed because the universe would enter a quantum phase [35]. Further consequences concern black holes in such a universe because no horizon and no singularity would ever form.

These considerations are certainly speculative. They demonstrate, however, that interesting consequences would result in quantum cosmology if the underlying equations were taken seriously.

Once the background (described by the scale factor and some other relevant variables) has assumed classical properties, the stage is set for the quantum-to-classical transition of the primordial fluctuations which serve as the seeds for structure formation. The interaction with further irrelevant degrees of freedom produces a classical behaviour for the field amplitudes of these fluctuations [36]. These, then, manifest themselves in the form of classical stochastic fluctuations that leave their imprint in the anisotropy spectrum of the cosmic microwave background radiation.

7 A panacea for cosmological singularities? — Singularity avoidance

As we have discussed above, a major motivation for the quantization of general relativity is the occurrence of singularities in generic physical models (but see [37, 38] for alternative views). This is why a touchstone of any quantum theory of gravity is its ability to remove these singularities in some (still to be specified) sense. In the cosmological context, the singularity of major concern is the big-bang singularity. But restriction to this singularity is far from exhausting even the possibilities offered by the most plain homogeneous, isotropic models. Related to dark energy is, for example, the big rip, a singularity occuring at large scale factor [28]. Another example of such a large-scale singularity is the big brake [39], see the subsection below.

First one should make up ones mind about whether quantum cosmology should resolve all conceivable singularities or just those which are physically motivated in the most conservative sense (e.g. big bang). Here it may help to fall back on quantum mechanics. The classical divergence of the Coulomb potential is removed through quantization. But nobody takes exception to the singularity persisting in quantum mechanics for the potential which falls off with the inverse squared distance, to mention one example. In quantum mechanics, singularity resolution is obviously restricted to the physically relevant cases. Even though these cases are much harder to make out in the cosmological context (as we are ignorant of the future of our Universe and partly even of the past), one should keep this in mind when discussing more exotic types of singularities.

Moreover, it is important to note that despite the very obvious importance of a criterion for singularity avoidance, no formal criterion for the avoidance of singularities on the quantum level exists by now. There are various different notions but, so far, no systematic scheme has developed. This lack of rigour is partly owed to an insufficient understanding of singularities already at the classical level.

7.1 Singularity avoidance of classical singularities defined through local criteria

The criterion which is most important for the identification of a cosmological singularity is the divergence of curvature scalars. Metrics which produce infinite curvature scalars are unphysical and therefore classified as singular. This is exactly the criterion applying to the big-bang singularity. It is a particularly useful criterion in quantum cosmology, for it relates the singularity definition directly to properties of the metric. This allows to mark singular regions in the space on which the wave function of the universe is defined. In homogeneous, isotropic cosmologies this is the point where the scale factor vanishes, $a = 0$. From this, one arrives quite intuitively at the following criterion for singularity avoidance on the quantum level:

Vanishing of the wave function

The singularity is avoided if the wave function vanishes on classically singular (in the sense that it produces diverging curvature invariants) three-metrics. This is perhaps the most intuitive and immediate way to think of singularity resolution. It may be the reason why it forms the content of the first boundary proposal in canonical quantum gravity put forward by DeWitt in 1967 [7]. Actually, this idea comes to mind so immediately that it is hard to support by arguments. Adding them nonetheless, one would say that regions of configuration space on which the wave function has no support are of no importance in quantum theory as every statement deduced from quantum theory employs the wave function. Of course, this is again a generalization of what we know from ordinary quantum theory. But it seems hard to argue that the role of the wave function in quantum theory is altered by the inclusion of gravity to the quantized interactions.[12] There are, in fact, several examples in the literature for singularity avoidance through vanishing wave function [42, 39].

In geometrodynamics, where the scale factor is restricted to be positive, the big-bang singularity lies at the boundary of configuration space. Vanishing of the wave function at the big bang is therefore often due to a certain type of boundary condition, see Section 4. Even more, the choice of boundary conditions might be justified from the strive for a singularity-free quantum theory [7, 10, 33]. (The situation is different in loop quantum cosmology where the big bang lies in the centre of configuration space due to the fact that here also negative values of the scale factor are allowed [17].)

It must, on the other hand, be emphasized that a non-vanishing, even a diverging, wave function does not necessarily entail a singularity: the ground-state wave function of the hydrogen atom (as found from the Dirac equation),

[12] Note that this statement does not touch upon the interpretation of the wave function nor upon the question of how information may be retrieved from the wave function. It just amounts to saying that the wave function is the fundamental building block of any quantum theory. For an alternative point of view see [41].

for example, diverges for $r \to 0$, but its norm stays finite due to a factor r^2 in the measure. Vanishing of the wave function can thus only be a sufficient, not a necessary criterion for singularity avoidance.

Well-defined quantum equations - Deterministic quantum evolution

An obvious prerequisite for this condition to be satisfied is that the equation describing the evolution of the wave function be well-defined — also at the singular metric. In the geometrodynamical picture this is obtained through the introduction of the variable $\alpha = \ln a$ which moves the big-bang singularity out to infinity. Loop quantum cosmology arrives at a finite evolution equation through a renormalization of the unbounded curvature terms. It is the fact that in loop quantum cosmology the big bang lies in the centre of configuration space that suggested to generalize this criterion to so-called 'quantum hyperbolicity' [41]. Quantum hyperbolicity asks for a deterministic evolution of general solutions to the constraint equations (Wheeler–DeWitt or the corresponding difference equation) through regions of classically singular metrics.

7.2 Singularity avoidance of classical singularities defined through global criteria

Not all singularities arise through a divergence of curvature invariants. In general relativity, a singularity is mathematically rigorously defined via geodesic incompleteness. We can therefore speak of singularities (or their avoidance) *only* when we have a notion of geodesics. This notion is tightly knit to the concept of spacetime. On the quantum-gravity level, spacetime is absent. We have three-metrics and their canonically conjugate momenta but no prescription how to stack these three-metrics together to obtain a four-dimensional spacetime (due to the uncertainty between the three-metric and its conjugate momentum, which is related to the extrinsic curvature). The recovery of spacetime structure is possible only in the semiclassical regime. Only here can we feasibly speak of spacetime and only here can we apply the geodesic equation, thus deciding about geodesic completeness or incompleteness. Thus one arrives at the appealing picture that incomplete geodesics lead into quantum regimes — their incompleteness being due to a break-down of the spacetime picture.

Break-down of the semiclassical approximation

Singularity avoidance is here equivalent to the statement that the semiclassical approximation breaks down in the region of the classical singularities. This criterion can be found in the early works by Hartle, Hawking and followers, see also [6] and the discussion above. Here, regimes where the wave function is a real exponential were denoted as classically forbidden. Only where the wave function in the semiclassical approximation was oscillatory, would one speak of a classically allowed region. This argumentation follows closely our knowledge from quantum mechanics where exponentially decaying wave functions occur in classically forbidden regions. Moreover, it is only out of oscillatory wave functions that one can form wave packets. But only tightly peaked wave packets allow the application of Ehrenfest's principle and the transition to a classical picture. Consequently, a spreading of wave packets can also be interpreted as a break-down of the semiclassical approximation [2, 34, 43, 28].

7.3 Example of singularity avoidance

An illustrative model is quantum cosmology with a big-brake singularity [39]. A big-brake singularity is a singularity where in the classical model both scale factor and its first time derivative stay finite, but the second derivative (the deceleration) diverges – the universe comes to a halt infinitely fast. What makes this model particularly interesting is the fact that the classical singularity occurs for big universes, that is, far away from the Planck scale where the usual big-bang singularity occurs.

The model describes a Friedmann universe with a scalar field that has no mass but a potential of a special form. The classical trajectory in configuration space is depicted in Figure 7. Upon discussing the Wheeler–DeWitt equation,

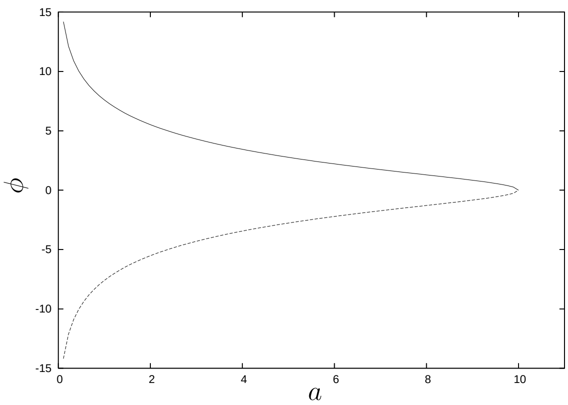


Fig. 7. Classical trajectory in configuration space [39]. Degrees of freedom are the scale factor a and scalar field ϕ. The singularity (big brake) is at $\phi = 0$.

one finds that all normalizable solutions lead to a wave function that *vanishes* at the point of the classical singularity; this we interpret as singularity avoidance. In Figure 8 we show a wave-packet solution that follows the classical trajectory and that vanishes at the classical singularity. An analogous situa-

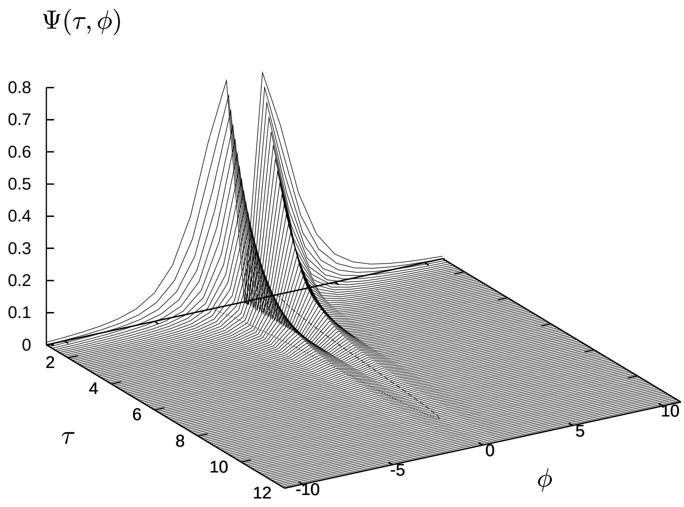


Fig. 8. This plot shows the wave packet. It follows classical trajectories with initial values $a_0 = 1$ and $\phi_0 \approx 0.88$. The classical trajectories are depicted in the (τ, ϕ)-plane, with $\tau = a^6$. From [39].

tion of singularity avoidance is found in the loop quantum cosmology of this model [39].

8 Concluding remarks

We have discussed that from a fundamental point of view it is important to deal with cosmology in quantum terms. This will cast light on many important issues such as the role of time, the origin and fate of the universe, the origin of irreversibility and structure, and the quantum measurement problem. All these were and are still pressing issues and opportunities which spur research in the field of quantum cosmology. Despite ongoing research and progress, many open questions remain. As the most important progress in quantum cosmology may consist in a better understanding of the questions and their relevance, we want to conclude our contribution by highlighting some of the most important questions in the field:

- How does one properly impose boundary conditions in quantum cosmology?
- Is the classical singularity being avoided?
- Will there be a genuine quantum phase in the future?
- How does the appearance of our classical universe follow from quantum cosmology?

- Can the arrow of time be understood from quantum cosmology?
- How does the origin of structure proceed?
- Is there a high probability for an inflationary phase? Can inflation itself be understood from quantum cosmology?
- Can quantum cosmological results be justified from full quantum gravity?
- Which consequences can be drawn from quantum cosmology for the measurement problem in quantum theory and for the field of quantum information?
- Can quantum cosmology be experimentelly tested?

Acknowledgements

We thank Alexander Vilenkin and Hongbao Zhang for their comments on our manuscript. B.S. thanks the Friedrich-Ebert-Stiftung for financial support.

A Derivation of the Wheeler–DeWitt equation for a concrete model

The starting point is the Einstein–Hilbert action of general relativity,

$$S_{\mathrm{EH}} = \frac{1}{2\kappa^2}\int \mathrm{d}^4x\sqrt{-g}(R-2\Lambda)\ , \tag{18}$$

where $\kappa^2 = 8\pi G$, R is the Ricci scalar, Λ denotes the cosmological constant, g stands for the determinant of the metric and integration is carried out over all spacetime. The general procedure of the canonical formulation and quantization was outlined in Section 2 and can be found in detail in, for example, [2, 18].

We want to apply the formalism for the case of a Friedmann universe, which is of central relevance for quantum cosmology. In the homogeneous and isotropic setting the line element is given by

$$ds^2 = -N(t)^2dt^2 + a(t)^2d\Omega_3^2\ , \tag{19}$$

where $d\Omega_3^2$ is the line-element of an constant curvature space with curvature index $k = 0, \pm 1$.

Here, N is the lapse function, measuring the change of coordinate time with respect to proper time. Setting $N = 1$ yields the conventional Friedmann time. This is a preferred foliation given for the isotropic and homogeneous setting by observers comoving with the cosmological perfect fluid.

The cosmological fluid shall here be mimicked by a scalar field ϕ with potential $V(\phi)$. The model is thus described by the action

$$
\begin{aligned}
S &= S_{\text{grav}} + S_{\text{matter}} \\
&= \frac{3V_0}{\kappa^2} \int dt N \left(-\frac{a\dot{a}^2}{N^2} + ka - \frac{\Lambda a^3}{3} \right) \\
&\quad + \frac{V_0}{2} \int dt N a^3 \left(\frac{\dot{\phi}^2}{N^2} - 2V(\phi) \right) .
\end{aligned} \tag{20}
$$

Here, V_0 is the volume of a spatial slice. In the following we choose, for convenience, $V_0 = 2\pi^2$ (assuming the three-space is a three-sphere). We thus have a Lagrangian system with two degrees of freedom, a and ϕ. The canonical momenta read

$$
\pi_a = \frac{\partial L}{\partial \dot{a}} = -\frac{6a\dot{a}}{\kappa^2 N} , \quad \pi_\phi = \frac{\partial L}{\partial \dot{\phi}} = \frac{a^3 \dot{\phi}}{N}, \quad \pi_N = \frac{\partial L}{\partial \dot{N}} \approx 0 . \tag{21}
$$

Curly equal signs stand for weak equalities, that is, equalities which hold after the equations of motion are satisfied. The equation for π_N is thus a primary constraint. The Hamiltonian reads

$$
\begin{aligned}
\mathcal{H} &= \pi_a \dot{a} + \pi_\phi \dot{\phi} + \pi_N \dot{N} - \mathcal{L} \\
&= -\frac{\kappa^2}{12a}\pi_a^2 + \frac{1}{2}\frac{\pi_\phi^2}{a^3} + a^3 \frac{\Lambda}{\kappa^2} + a^3 V - \frac{3ka}{\kappa^2} .
\end{aligned} \tag{22}
$$

As we assumed homogeneity and isotropy, the diffeomorphism constraints are satisfied trivially. From the preservation of the primary constraint $\pi_N \approx 0$ one finds that the Hamiltonian is constrained to vanish, $\mathcal{H} \approx 0$. Expressed in terms of the 'velocities', $\dot{a}$ and $\dot{\phi}$, this constraint becomes identical to the Friedmann equation,

$$
\left(\frac{\dot{a}}{a} \right)^2 \equiv H^2 = \frac{\kappa^2}{3} \left(\frac{\dot{\phi}^2}{2} + V(\phi) \right) + \frac{\Lambda}{3} - \frac{k}{a^2} . \tag{23}
$$

The space spanned by the canonical variable (the three-metric) in the full theory is called superspace, see the main text. In dependence on this denotation, the space spanned by (a, ϕ) is called minisuperspace. The metric on this space is named after DeWitt and is for this model given by

$$
G_{AB} = \begin{pmatrix} -\frac{6a}{\kappa^2} & 0 \\ 0 & a^3 \end{pmatrix} . \tag{24}
$$

Note the indefinite nature of the metric, resulting in an indefinite DeWitt metric for general relativity. The Hamiltonian constraint in this minisuperspace model thus reads

$$
\mathcal{H} = N \left(\frac{1}{2} G^{AB} \pi_A \pi_B + \mathcal{V}(q) \right) \approx 0 , \tag{25}
$$

where

$$\mathcal{V}(q) = \frac{1}{2}\left(-\frac{6ka}{\kappa^2} + \frac{2\Lambda a^3}{\kappa^2} + a^3 V(\phi)\right) , \tag{26}$$

$A, B = \{a, \phi\}$, that is, $q^1 = a, q^2 = \phi$, and G^{AB} is the inverse DeWitt metric. It is an artefact of the two-dimensionality of the model considered here that minisuperspace is conformally flat. In more complicated settings, minisuperspace can also be curved and additional curvature terms may occur depending on the choice of factor ordering.

Dirac's constraint quantization requires an implementation of (22) as

$$\hat{\mathcal{H}}\Psi = 0 . \tag{27}$$

The operator $\hat{\mathcal{H}}$ is constructed from the conventional Schrödinger representation of canonical variables,

$$\hat{q}_A \Psi \equiv q_A \Psi , \qquad \hat{\pi}_A \Psi \equiv \frac{\hbar}{\mathrm{i}} \frac{\partial}{\partial q_A} \Psi , \tag{28}$$

for $A \in \{a, \phi\}$. Of course, the Hamiltonian operator is not uniquely defined in this way. On the contrary, factor-ordering ambiguities occur here as in ordinary quantum mechanics — with the important difference that factor ordering can here not be justified by experiment. Usually one decides on the covariant ordering, the Laplace–Beltrami ordering,

$$G^{AB}\pi_A\pi_B \to -\hbar^2 \nabla^2_{\mathrm{LB}} = -\frac{\hbar^2}{\sqrt{-\mathcal{G}}}\partial_A\left(\sqrt{-\mathcal{G}}G^{AB}\partial_B\right) , \tag{29}$$

where $\mathcal{G}$ denotes the determinant of the DeWitt–metric. Choosing Laplace–Beltrami factor ordering, the Wheeler–DeWitt equation reads

$$\left(\frac{\hbar^2\kappa^2}{12} a\frac{\partial}{\partial a} a\frac{\partial}{\partial a} - \frac{\hbar^2}{2}\frac{\partial^2}{\partial\phi^2} + a^6\left(V(\phi) + \frac{\Lambda}{\kappa^2}\right) - \frac{3ka^4}{\kappa^2}\right)\Psi(a,\phi) = 0 . \tag{30}$$

Introducing $\alpha \equiv \ln a$, one obtains the following equation

$$\left(\frac{\hbar^2\kappa^2}{12}\frac{\partial^2}{\partial\alpha^2} - \frac{\hbar^2}{2}\frac{\partial^2}{\partial\phi^2} + e^{6\alpha}\left(V(\phi) + \frac{\Lambda}{\kappa^2}\right) - 3e^{4\alpha}\frac{k}{\kappa^2}\right)\Psi(\alpha,\phi) = 0 . \tag{31}$$

This is an equation of the same form as the Klein–Gordon equation: the derivative with respect to α corresponds to a time derivative, the derivative with respect to ϕ to a spatial derivative, and the remaining terms constituting a 'time and space dependent' mass term, that is, a non-trivial potential term. Equation (31) is the starting point for many discussions in quantum cosmology. The physical units are often chosen to be $\kappa^2 = 6$ for convenience.

References

1. E. Joos, H. D. Zeh, C. Kiefer, D. Giulini, J. Kupsch, and I.-O. Stamatescu (2003): *Decoherence and the Appearance of a Classical World in Quantum Theory*, second edition (Springer, Berlin).

2. C. Kiefer (2007): *Quantum Gravity*, second edition (Oxford University Press, Oxford).
3. C. Kiefer (2006): Quantum cosmology: expectations and results. *Annalen der Physik* **15**, 316–325.
4. D. H. Coule (2005): Quantum cosmological models. *Class. Quantum Grav.* **22**, R125–166.
5. D. L. Wiltshire (1996): An introduction to quantum cosmology. In: *Cosmology: The physics of the Universe*, edited by B. Robson, N. Visvanathon, and W. S. Woolcock (World Scientific, Singapore), pp. 473–531.
6. J. J. Halliwell (1991): Introductory lectures on quantum cosmology. In: *Quantum Cosmology and Baby Universes*, edited by S. Coleman, J. B. Hartle, T. Piran, and S. Weinberg (World Scientific, Singapore), pp. 159–243.
7. B. S. DeWitt (1967): Quantum theory of Gravity. I. The canonical theory. *Phys. Rev.* **160**, 1113–1148.
8. C. W. Misner (1972): Minisuperspace. In: *Magic without magic*, edited by J. R. Klauder (Freeman, San Francisco), pp. 441–473.
9. M. P. Ryan (1972): *Hamiltonian Cosmology.* Lecture Notes in Physics **13** (Springer, Berlin).
10. J. B. Hartle and S. W. Hawking (1983): Wave function of the Universe. *Phys. Rev. D* **28**, 2960–2975.
11. A. Vilenkin (1982): Creation of universes from nothing. *Phys. Lett. B* **117**, 25–28.
12. A. Vilenkin (2003): Quantum cosmology and eternal inflation. In: *The future of theoretical physics and cosmology*, edited by G. W. Gibbons *et al.* (Cambridge University Press, Cambridge), pp. 649–666.
13. H. D. Conradi and H. D. Zeh (1991): Quantum cosmology as an initial value problem. *Phys. Lett. A* **154**, 321–326.
14. A. O. Barvinsky (2001): Quantum cosmology at the turn of millenium; `gr-qc/0101046`.
15. M. Gasperini and G. Veneziano (2003): The pre-big bang scenario in string cosmology. *Phys. Rep.* **373**, 1–212; M. P. Dąbrowski and C. Kiefer (1997): Boundary conditions in quantum string cosmology. *Phys. Lett. B* **397**, 185–92.
16. P. V. Moniz (1996): Supersymmetric quantum cosmology – shaken, not stirred. *Int. J. Mod. Phys. A* **11**, 4321–4382.
17. A. Ashtekar and M. Bojowald, contribution to this volume.
18. D. Giulini and C. Kiefer (2007): The canonical approach to quantum gravity – general ideas and geometrodynamics. In: *Approaches to fundamental physics – An assessment of current theoretical ideas*, edited by E. Seiler and I.-O. Stamatescu (Springer, Berlin), pp. 131–150.
19. R. Arnowitt, S. Deser, and C. W. Misner (1962): The dynamics of general relativity. In: *Gravitation: an introduction to current research*, edited by L. Witten (Wiley, New York), pp. 227–265.
20. C. Rovelli (2004): *Quantum Gravity* (Cambridge University Press, Cambridge).
21. J. Klauder (2006): Fundamentals of quantum gravity; `gr-qc/0612168`.
22. C. J. Isham (1992): Canonical quantum gravity and the problem of time; `gr-qc/9210011`.
23. K. Kuchař (1992): Time and interpretations of quantum gravity. In: *Proc. 4th Canadian Conf. General Relativity and Relativistic Astrophysics*, edited by G. Kunstatter *et al.* (World Scientific, Singapore), pp. 211–314.

24. C. G. Torre (1993): Is general relativity an 'already parametrized' theory? *Phys. Rev. D* **46**, 3231–3234.
25. R. F. Baierlein, D. H. Sharp, and J. A. Wheeler (1962): Three-dimensional geometry as carrier of information about time. *Phys. Rev.* **126**, 1864–1865.
26. H. D. Zeh (1988): Time in quantum gravity. *Phys. Lett. A* **126**, 311–317.
27. C. Kiefer (1989): Non-minimally coupled scalar fields and the initial value problem in quantum gravity. *Phys. Lett. B* **225**, 227–232.
28. M. P. Dąbrowski, C. Kiefer, and B. Sandhöfer (2006): Quantum phantom cosmology. *Phys. Rev. D* **74**, 044022.
29. H. D. Conradi (1998): Tunneling of macroscopic universes. *Int. J. Mod. Phys. D* **7**, 189–200.
30. C. Kiefer and T. P. Singh (1991): Quantum gravitational correction terms to the functional Schrödinger equation. *Phys. Rev. D* **44**, 1067–1076; A. O. Barvinsky and C. Kiefer (1998): Wheeler–DeWitt equation and Feynman diagrams. *Nucl. Phys. B* **526**, 509–539; C. Kiefer, T. Lück, and P. Moniz (2005): Semiclassical approximation to supersymmetric quantum gravity. *Phys. Rev. D* **72**, 045006.
31. C. Kiefer, J. Marto, and P. V. Moniz (2008): Canonical quantum gravity and black hole evaporation. In preparation.
32. J. J. Halliwell and S. W. Hawking (1985): Origin of structure in the Universe. *Phys. Rev. D* **31**, 1777–1791.
33. A. Vilenkin (1989): Interpretation of the wave function of the Universe. *Phys. Rev. D* **39**, 1116–1122.
34. H. D. Zeh (2007): *The physical basis of the direction of time*, fifth edition (Springer, Berlin).
35. C. Kiefer and H. D. Zeh (1995): Arrow of time in a recollapsing quantum universe. *Phys. Rev. D* **51**, 4145–4153.
36. C. Kiefer, D. Polarski, and A. A. Starobinsky (1998): Quantum-to-classical transition for fluctuations in the early universe. *Int. J. Mod. Phys. D* **7**, 455–462.
37. B. Mashhoon (2001): Gravitation and non-locality. In: *Proceedings of the 25th Johns Hopkins Workshop 2001: A Relativistic Spacetime Odyssey* (World Scientific, Singapore), pp. 35–46.
38. D. A. Konkowski, T. M. Helliwell, and V. Arndt (2004): Are classically singular spacetimes quantum mechanically singular as well? In: *Proceedings of the Tenth Marcel Grossmann Meeting on General Relativity, Rio de Janeiro* (World Scientific, Singapore), pp. 2169–2171.
39. A. Y. Kamenshchik, C. Kiefer, and B. Sandhöfer (2007): Quantum cosmology with a big-brake singularity. *Phys. Rev. D* **76**, 064032.
40. S. W. Hawking and G. F. R. Ellis (1973): *The large scale structure of space–time*. Cambridge University Press, Cambridge.
41. M. Bojowald (2007): Singularities and quantum gravity; `gr-qc/0702144`.
42. H. D. Conradi (1995): Quantum cosmology of Kantowski-Sachs like models. *Class. Quantum Grav.* **12**, 2423–2439.
43. C. Kiefer (1988): Wave packets in minisuperspace. *Phys. Rev. D* **38**, 1761–1772.