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A STUDY OF THE PROBLEM OF TIME IN A FRIEDMANN QUANTUM COSMOLOGY

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Abstract

After reviewing Dirac's canonical quantization program and the canonical quantization of General Relativity, we study the problem of time in the context of a quantum minisuperspace cosmological model: a Friedmann-Lemaître-Robertson-Walker spacetime coupled minimally to a scalar field. We explore different methods to include time and evolution in our formalism. We begin by discussing the possibility to identify a dynamical time variable before quantization. Such a time variable is constructed as a function of the phase space variables and leads to a multiple choice problem for the evolution of our quantum system. We then explore the connection between the Born-Oppenheimer approach to the problem of time and gauge fixing. We find that by choosing a particular gauge we can recover the Born-Oppenheimer approach ansatz both in the classical and in the quantum theory. In the latter, the result of the BO approach is recovered by performing a phase transformation in the Wheeler-DeWitt equation and requiring that the resulting Schrödinger-like equation is unitary.

Abstract

Dopo una rassegna del programma di Dirac per la quantizzazione canonica della relatività generale, studiamo il problema del tempo nel contesto di un modello cosmologico dato da un minisuperspazio quantistico: uno spaziotempo Friedmann-Lemaître-Robertson-Walker con accoppiamento minimale ad un campo scalare. Esploriamo diversi metodi per includere il tempo e l'evoluzione temporale nel nostro formalismo. Iniziamo discutendo la possibilità di identificare una variabile temporale dinamica prima della quantizzazione. Una tale variabile temporale è costruita come funzione delle variabili dello spazio delle fasi e conduce a delle ambiguità nell'evoluzione temporale. Successivamente esploriamo la connessione tra l'approccio di Born-Oppenheimer al problema del tempo e il fissare un gauge. Troviamo che scegliendo un gauge apposito si ritrova l'ansatz dell'approccio di Born-Oppenheimer sia nella teoria classica che in quella quantistica. In quest'ultima, il risultato dell'approccio di Born-Oppenheimer è ottenuto anche effettuando una trasformazione di fase nell'equazione di Wheeler-de Witt richiedendo che la risultante equazione di tipo Schrödinger sia unitaria.

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Introduction

The understanding of the concept of time is one of the deepest gaps in our current knowledge of the universe. The fascination and uncertainty in the meaning of this concept can be summarized in the words of Saint Augustine, who said, as early as 389 A.D, the following words [1]:

> "*What then is time? If no one asks me, I know what it is. If I wish to explain it to him who asks, I do not know.*"

This quest to understand what time is and the role that it plays in our universe is particularly interesting in physics, where the concept of an absolute time that is continuous, infinite and can be used to describe the dynamics of all bodies and all laws of physics was established by Newton's Laws of Mechanics [2].

The view of time like a parameter external to our systems was challenged by the developments of special and General Relativity. In these theories, time and space are treated on equal footing, meaning that time is not anymore absolute, but it is dynamic. In the particular case of Minkowski spacetime in special relativity, the division of spacetime into space and time is more of an useful choice we make and is not inherent to the physical situations themselves [3].

Another important characteristic of these theories is that in both, special and General Relativity, equations transform covariantly under changes of spacetime coordinates. This means that for a quantity to be considered "physical" it should be independent of the choice of coordinates [4]. In the case of special relativity, the equations are covariant under the action the the Poincaré group, while in the case of General Relativity the Poincaré group is substituted by the more general group diff($\mathcal{M}$), which is the group of diffeomorphisms of the spacetime manifold $\mathcal{M}$ [2, 3, 4].

In this context, General Relativity can be regarded as a Gauge theory. There are other very important and successful theories of this kind, for example, we can mention electrodynamics and Yang-Mills theory[1], which form the base of our understanding of the Standard Model (SM) of particle physics.

[1]String and superstring theories are other popular examples that share with General Relativity the fundamental feature that they are reparametrization invariant.

The Standard Model has been very successful in the sense that results from high energy physics experiments performed at colliders (and more specifically, at the Large Hadron Collider, at CERN) can be explained by this theory. However, there are different hints that tells us that the SM is incomplete [5]. One of these issues is precisely that in the SM three forces of nature (electromagnetism, weak and the strong force) are described at a quantum level, while gravity is only treated classically.

Since all the forces in the Standard Model are described by Gauge theories and we have argued that General Relativity is also a theory of this kind, we could hope that an approach analogous to the one made for Yang-Mills and electromagnetism would suffice to include General Relativity in the Standard Model. However, when we look at the gauge groups of General Relativity and Yang-Mills, we realize that they are analogous in the sense that in both cases they are associated with a canonical formalism that produces constraints on the canonical variables, but the analogy ends when we notice that Yang-Mills transformations occur at a particular point in spacetime, while the invariance under the diffeomorphism group implies that individual points in our manifold $\mathcal{M}$ have no fundamental significance [4]. For example, the value of a scalar field in a particular point x of our manifold has no invariant meaning.

This raises the questions of what is really an observable in General Relativity. Before, we mentioned that for a quantity to be consider physical, it should be independent of the choice of coordinates. This idea carries with it some questions that are of particular interest to us. The first of them has to do with the fact that time is usually regarded as a coordinate on our manifold $\mathcal{M}$, so, we should expect that it plays no fundamental role in our theories. But if time has no physical significance, how does *change* emerge in our formalism?

A second, but not less important question is if this view is compatible with the notion of time in quantum mechanics. The answer is, in principle, that the two notions are not compatible. This incompatibility has its heart in the special role that time plays in the quantum theory: time is not represented by an operator, but it is instead a background parameter, external to the system. In other words, the concept of time used in conventional quantum theory is the Newtonian one. [4]

This incompatibility is known as “The Problem of Time” and turns out to be the source of serious problems in the search for a quantum theory of gravity [6]. To understand why, we need to take a look at the canonical approach to quantum gravity (see, for example, [7]). After performing the $3+1$ decomposition of the Einstein-Hilbert action, defining canonical variables and identifying the primary constraints (for a review of Dirac's canonical quantization program see [8]), we can write the Hamiltonian

$$H_D = \int d^3x (N^\alpha \mathcal{H}_\alpha + N\mathcal{H}). \tag{1}$$

Here, N and N_α are called the lapse function and the shift vector and $\mathcal{H}$, $\mathcal{H}_\alpha$ are the super Hamiltonian and the super momentum, correspondingly.

The super Hamiltonian and the super momentum are constrained to vanish weakly:

$$\mathcal{H}_\alpha \approx 0, \qquad\qquad \mathcal{H} \approx 0. \tag{2}$$

Then, we can see that also our Hamiltonian will vanish weakly, because it is a linear combination of the constraints. Since the Hamiltonian governs the quantum dynamics, the fact that it vanishes means that we can't write a time dependent Schrödinger equation. In other words, our quantum states will appear to be "frozen".

More specifically, upon quantization both the super Hamiltonian and the super momentum must be turned into operators:

$$\mathcal{H}_\alpha \longrightarrow \hat{\mathcal{H}}_\alpha, \qquad\qquad \mathcal{H} \longrightarrow \hat{\mathcal{H}}. \tag{3}$$

These operators act on our quantum state $|\psi\rangle$. The equation for the momentum constraint, $\hat{\mathcal{H}}_\alpha |\psi\rangle = 0$, is automatically satisfied if $|\psi\rangle$ is invariant under coordinate transformations, which is consistent with the fact that the momentum constraint can be interpreted as the generator of diffeomorphisms in our hypersurfaces [9].

On the other hand, the quantum dynamics is actually governed by the Hamiltonian constraint, and the equation

$$\hat{\mathcal{H}} |\psi\rangle = 0 \tag{4}$$

is known as the Wheeler-DeWitt equation [10]. The interpretation of this equation in physical terms remains an open question. In particular, the apparent absence of time and, as a consequence, of evolution of the states must be accounted for somehow. However, equation (4) remains as the basis of different approaches to quantum gravity and quantum cosmology.

Actually, quantum cosmology plays a fundamental role in the study of quantum gravity, since cosmological models are simple examples to which the ideas of a quantum theory of gravity may be applied in order to extract meaningful results that could be confronted with observational data.

In principle, the goal of quantum cosmology is to describe the universe in its very early stages and provide initial conditions for inflation, i.e. of the stage of the history of the very early universe when it undergoes a very rapid quasi-exponential expansion. Quantum gravity effects are expected to have played an important role during this period, leaving a print in the cosmological fluctuations produced during inflation that may be observable in the cosmic microwave background [11].

However, the full formalism of quantum cosmology is very difficult to deal with in practice, since the configuration space is infinite dimensional. Here is where the concept of *minisuperspace* comes into play. Minisuperspaces are a particular class of models that have a finite dimensional configuration space. Much of the work done in quantum cosmology has concentrated on models of this type.

Minisuperspaces are characterized by the imposition of symmetries in the metric in order to get a theory with a finite number of degrees of freedom. Examples of these type of cosmologies are Firedmann-Lemaître - Robertson-Walker (FLRW) models, the Bianchi-type spacetimes and Kantowski - Sachs universe.

These models share relevant features with the full theory. In particular, the problem of time is present in the cosmologies mentioned above. So, studying how to solve the problem of time in this context is not only simpler, but it can give us great insight into the full theory of quantum gravity, while at the same time allowing us to get some useful predictions about quantum gravity effects that might have played an important role during inflation. These predictions could in principle be confronted with observational data of the cosmic microwave background.

Taking what we have discussed into consideration, we can ask the following question: how can we reintroduce the notion of time and evolution in a quantum theory of gravity, in particular in the context of quantum cosmology and minisuperspaces? The present thesis project deals with this question.

This work is divided into six chapters. In chapter I and II, we review Dirac's canonical quantization program and the canonical quantization of General Relativity, which are the basis of the study of the problem of time. In chapter III we discuss the problem of time in more detail, including the different approaches that have emerged through the years and the technical problems that appear while trying to solve it.

In chapter IV, we perform the canonical quantization of a flat FLRW spacetime coupled to a scalar field. This minisuperspace model will be our subject of study in the following two chapters.

Chapter V is dedicated to the study of the problem of time in the quantum minisuperspace of chapter IV. We attempt to identify time before quantization using a method described in [12]. Finally, chapter VI is dedicated to the study of the connection between the Born-Oppenheimer approach to the problem of time and the gauge fixing approach.

In the words of Isham[4]: "the problem of 'time' is one of the deepest issues that must be addressed in the search for a coherent theory of quantum gravity." This sentence summarizes the importance that solving this problem has for theoretical physics and, on a deeper level, for the foundations of physics. A better understanding of its different aspects, which can be achieved through the study of simpler models like minisuperspaces, can help us construct one of the missing pieces in our modern understanding of the universe: a quantum theory of gravity, which has been elusive up to now.

Chapter 1

Dirac's canonical quantization program

Theories with constraints have been very successful in describing nature [13]. As examples of these kind of theories we can mention electrodynamics and Yang-Mills theory, which form the basis of our understanding of the Standard Model (SM) of particle physics. Another very important example of a theory with constraints is General Relativity, which is the only one of the four fundamental forces of nature that it's not included in the Standard Model [5].

In all the cases mentioned before we start with a classical theory, which is then quantized using canonical quantization [8]. The method to construct a quantum theory beginning from a classical theory with constraints was established by Dirac as is known as Dirac's canonical quantization program [14], which we now proceed to describe.

To get a feeling for Dirac's procedure we first review the usual Hamiltonian description of a system. Consider a system described by a set of coordinates q^i, where $i = 1, ..., n$. The q^i are coordinates on a manifold and this manifold is called the configuration space.

The evolution of the system can be thought as a path in the configuration space [8]. This path can be described by the function $\vec{q}(t)$, where t is the time variable and $\vec{q}$ denotes a point in the configuration space. Such a path is called the evolution of the system.

The dynamic of the system is described by the action. The physical path that our system follows is the one that extremises the action [15], defined as follows:

$$S[q(t)] = \int dt L(q(t), \dot{q}(t)).$$

Here $L(q(t)), \dot{q}(t)$ is the Lagrangian of the system. By performing variations in the action we can derive the equations of motion, which are given by the well-known Euler-Lagrange equations [15]:

$$\frac{\partial L}{\partial q^i}(q,\dot{q}) = \frac{d}{dt}\frac{\partial L}{\partial \dot{q}^i}(q,\dot{q})$$

In general these are second order differential equations. We can turn them into a system of first-order differential equations by introducing an additional variable for each q^i. We'll call these new variables the conjugate momenta p_i. For each q^i, its conjugate momenta is defined as [8]:

$$p_i(t) = \frac{\partial L}{\partial \dot{q}^i}(q,\dot{q}), \qquad \dot{p}_i(t) = \frac{\partial L}{\partial q^i}(q,\dot{q}).$$

The time evolution is now given by the space spanned by the coordinates q^i and p_i. This space is called the *phase space*. A point in the phase space is called a state of the system.

On the phase space, we can introduce the Hamiltonian of the system [16]:

$$H(q,p) = p_i\dot{q}^i - L(p,\dot{q}). \tag{1.1}$$

Using the Hamiltonian we can rewrite the action as

$$S = \int dt\; p_i\dot{q}^i - H(q,p). \tag{1.2}$$

The corresponding equations of motion associated to this action are the Hamilton equations [16]:

$$\dot{q}^i(t) = \frac{\partial H}{\partial p_i}(q,p), \qquad \dot{p}_i(t) = -\frac{\partial H}{\partial q^i}(q,p).$$

The Hamilton equations describe the evolution of a state in the phase space and are equivalent to the Euler-Lagrange equations [8]. The time evolution of a function $F(p,q)$ on the phase space is given by its *Poisson bracket* with the Hamiltonian, defined as:

$$\dot{F}(p(t),q(t)) = \{F,H\} = \frac{\partial F}{\partial q^i}\frac{\partial H}{\partial p_i} - \frac{\partial H}{\partial q^i}\frac{\partial F}{\partial p_i}$$

Then, the dynamics of our system is completely determined by the Hamiltonian and the Poisson bracket [16]. However, to be able to write the Hamiltonian as equation (1.1) we have to solve the condition

$$p_i = \frac{\partial L}{\partial q^i}. \tag{1.3}$$

If this condition cannot be solved, it means two things [8]:

- The Hamiltonian can't be defined in this point of the phase space.
- There is no solution to the equations of motion passing through this point.

The fact that there is no solution to the equations of motion in a particular point of the phase space tells us that we don't really need the Hamiltonian there, since it is not part of the physical solutions of our systems. So, our Hamiltonian is well-defined only on the subspace of the phase space given by the image of the momentum map [13], equation (1.3).

The image of this map can be described by a set of equations $\psi_\alpha(q,p) = 0$, which we'll call *primary constraints*. The subspace of the phase space defined by the primary constraints is called the *primary constraint surface* [14].

Since we know that all the solutions of our system lie in the primary constraint surface and that the Hamiltonian is well defined there, we can rewrite the action (1.2) to include the restriction that the path has to lie in the primary constraint surface. We can do this by adding Lagrange multipliers to the action in the following way:

$$\tilde{S}[q,p,u] = \int dt\, \dot{q}^i p_i - H_0(q,p) - u^\alpha \psi_\alpha(q,p).$$

We can define the combination

$$H(q,p) = H_0(q,p) + u^\alpha \psi_\alpha \tag{1.4}$$

to be the Hamiltonian, so that the equations of motion now are

$$\psi_\alpha = 0, \qquad \dot{q}^i = \frac{\partial H}{\partial p_i}, \qquad \dot{p}_i = -\frac{\partial H}{\partial q^i}.$$

However, as we integrate our system we are going to find that it is not enough to start with a state in the primary constraint surface to remain on it, because in general states tend to evolve away from it [8]. So, we need to add the additional requirement that the constraints be satisfied at all times.

This requirement will impose more restrictions on the initial conditions of our system and will define another subspace of the the phase space. We call these additional restrictions *secondary constraints* and the smaller subspace that they define *the constraint surface*. Once we found all the constraints and start with a state solving them, we will stay in the constraint surface at all times [14].

Note that to derive the equations of motion we need the derivatives of the Hamiltonian, so we are free to add anything to it that vanishes and whose gradient vanishes in the constraint surface. With this idea in mind we can introduce the concept of *weak equality* [13].

Two phase space functions $F(q,p)$ and $G(q,p)$ are defined to be weakly equal if they coincide on the constraint surface. Weak equalities are denoted by the symbol $\approx$ and are not compatible with the Poisson bracket [8]. This means that if we have three phase space functions, $F(p,q)$, $G(p,q)$, $K(p,q)$, and we know that $F \approx G$, this doesn't necessarily implies $\{F,K\} \approx \{G,K\}$.

To summarize, the equations of motion can be derived from a Hamiltonian that takes the form (1.4). Where the ψ_α are the primary constraints and the u^α are the Lagrange multipliers that, in general, can be a set of phase space functions with some free parameters. To find the initial states that are allowed we need to require that also the time derivative of the primary constraint vanishes.

It is enough to ask that the time derivative of the primary constraints vanishes weakly [8], since this will ensure that the state remains in the constraint surface. So, we have to consider the following conditions:

$$\dot{\psi}_\alpha = \{\psi_\alpha, H\} \approx \{\psi_\alpha, H_0\} + u^\beta\{\psi_\alpha, \psi_\beta\} \approx 0 \tag{1.5}$$

Equation (1.5) represents a set of equations, some of which are the secondary constraints and some of which restrict the u^α's weakly. Of course, we also need to ask that the newly found secondary constraints be conserved under time evolution, so we have to evaluate (1.5) again for them, possibly getting more constraints. We have to keep repeating this procedure until we either find a contradiction, in which case there are no solutions to the equations of motion, or the new conditions are trivial [14].

In the second case, we end with a full set of constraints which define the constraint surface and the Hamiltonian takes the form (1.4), where we are now summing over both the primary and secondary constraints.

We mentioned before that the u^α are fixed only weakly and that they may contain some free parameters. We can now ask if after completing the procedure just described there will still be any free parameters left. To answer this question, remember that the u^α have to satisfy the following set of equations:

$$\{H_0, \psi_\alpha\} + u^\beta\{\psi_\alpha, \psi_\beta\} \approx 0. \tag{1.6}$$

Whether or not there are free parameters in the u^α depends on the matrix

$$\Delta_{\alpha\beta} = \{\psi_\alpha, \psi_\beta\}.$$

If this matrix is invertible, we can solve (1.6) [8], which will give us a weakly unique solution for all u^α. On the other hand, if this matrix is not invertible we will have some zero eigenvectors. We can then assume that there are a subset of constraints ϕ_a that have weakly vanishing Poisson bracket with all constraints:

$$\{\phi_a, \psi_\alpha\} \approx 0.$$

It is clear that in this case, equation (1.6) doesn't impose any restriction on the corresponding u^a.

We will now define a *first class function* as a phase space function that has weakly vanishing Poisson bracket with all the constraints. In this sense, the ψ_a are called the *first class constraints* [13].

The remaining constraints will be denoted by χ_m. Since the χ_m don't have vanishing Poisson bracket, the submatrix $\Delta_{mn} = \{\chi_m, \chi_n\}$ is invertible, meaning that the corresponding u^m are weakly fixed. We call the χ_m *second class constraints* [13].

Gauge transformations appear in this context as a term in the Hamiltonian proportional to the constraint multiplied by a free parameter. This means that if $F(q,p)$ is a phase space function, then

$$\delta F = u^a\{F, \phi_a\} \approx \{F, u^a\phi_a\}$$

gives the transformation of F generated by $u^a\phi_a$. In our case, the constraints that appear in this way in the Hamiltonian are the primary first class constraints, which lead us to the conclusion that these are the generators of gauge transformations [8]. It can be proven that also the secondary first class constraints generate gauge transformations.

Since we are free to perform gauge transformations at any time, we can add any linear combinations of first class constraints to our Hamiltonian. So, its final form will be

$$H(q,p,t) = H_0(q,p) + u^a(q,p,t)\phi_a(q,p).$$

The second class constraints are included into H_0 since they don't contain free parameters. The parameters in the case of the first class constraints can be any phase space function that can also depend on time.

The complete set of equations of motion will be

$$\phi_a(q,p) = 0, \qquad\qquad \chi_m(q,p) = 0.$$

That correspond to the first and second class constraints and the Hamilton equations:

$$\dot{q}^i = \frac{\partial H}{\partial p^i}, \qquad\qquad \dot{p}_i = \frac{\partial H}{\partial q^i}.$$

In the bracket notation, this can be written as

$$\dot{F}(q,p) = \{F, H\} \approx \{F, H_0\} + u^a\{F, \phi_a\}.$$

This last equation tells us that the time evolution is split into a "physical evolution" plus a gauge transformation.

Let us now briefly define observables in the context of constrained systems. For unconstrained systems observables are usually defined as phase space functions that can be measured. For constrained systems, a quantity that can be measured should be a function only on the constraint surface, since the states that are realized physically live there. Also, if we have a gauge symmetry, only those quantities invariant under the Gauge transformation can be defined as observables [8, 17].

We explained before that Gauge transformations are generated by the first class constraints. An observable must be invariant under Gauge transformations, which means it must have weakly vanishing Poisson bracket with the first class constraints:

$$\{O, \phi_a\} \approx 0.$$

This completes the classical part of Dirac procedure to describe the dynamics of constrained systems. Let's study now the more interesting quantum part.

1.1 Quantization of constrained systems

Before dealing with constrained systems let us review the canonical quantization procedure for an unconstrained system, which usually goes as follows [18]:

- Take the configuration space variables and their conjugate momenta and promote them to operators in some Hilbert space. A state will be represented as a vector of this Hilbert space.
- Substitute the Poisson bracket with the commutator between operators.
- Take the state space to be the set of square integrable complex wave functions Ψ on the configuration space and choose a representation for the operators:

$$\hat{q}\Psi(q) = q\Psi(q), \qquad \hat{p}\Psi(q) = -i\hbar\frac{\partial\Psi}{\partial q}(q).$$

- Impose the Schrödinger's equation, that in the Schrödinger's picture reads:

$$i\hbar\frac{d}{dt}|\Psi\rangle = \hat{H}|\Psi\rangle.$$

- Define the scalar product between two wave functions $|\Psi\rangle$ and $|\phi\rangle$ as

$$\langle\phi|\Psi\rangle = \int dq\ \phi^*(q)\Psi(q). \tag{1.7}$$

We can calculate expectation values of observables:

$$\langle\hat{F}\rangle = \langle\Psi|\,\hat{F}\,|\Psi\rangle\,.$$

Additionally, we have Ehrenfest's theorem, that tells us that expectation values of observables behave almost like the classical phase space functions.

Almost all these steps can also be defined in the case of a constrained system. But what about the constraints? We have argued that the constraints impose conditions on the initial states of our system and define the constraint surface, that in the phase space represents the possible physical states of our system.

On this line of thought, at the quantum level, we can promote the classical constraints to operators and think about them as restrictions to be imposed in the states $|\Psi\rangle$ [14]. The conditions to be imposed on a state are then

$$\hat{\psi}_\alpha\,|\Psi\rangle = 0.$$

In the last equation, $\hat{\psi}_\alpha$ are the quantum constraint operators. The states $\hat{\psi}_\alpha\,|\Psi\rangle$ are called physical states and they form a linear subspace that we call the physical state space [8].

To define observables in the quantum theory, we should remember that in the classical theory, they are defined as those phase space functions that have weakly vanishing Poisson bracket with the constraints. We will introduce a similar concept in the quantum theory making use of the commutator instead of the Poisson bracket. We will define a quantum observable $\hat{O}$ as an operator that commutes weakly with all constraints [14]:

$$[\hat{O},\hat{\phi}_a] \approx 0.$$

The fact that the commutator of an observable with all constraints vanishes weakly tells us that the observable maps physical states onto physical states, since

$$\hat{\phi}_a\hat{O}\,|\Psi\rangle = \hat{O}\hat{\phi}_a\,|\Psi\rangle - [\hat{O},\hat{\phi}_a]\psi = 0.$$

In general, for a constrained system, the product given in equation (1.7) will not give a suitable scalar product for the physical states [8]. So, if we are going to define a proper Hilbert space we should define a new scalar product.

The definition of the product is the last step of the quantization program and there is really no general rule to tell us how to do it [19]. The only condition that can help us identify the product is that we require that real observables become Hermitian operators.

Chapter 2

Canonical quantum gravity

Our goal in this chapter is to use Dirac's Canonical quantization program to perform the canonical quantization of General Relativity. In order to do this we need to write the Einstein-Hilbert action in a suitable form that will allow us to define canonical variables and their conjugates that will later be used to write the theory in Hamiltonian form.

Writing the action in "suitable form" means that to write the theory in Hamiltonian form we need to break the covariance of the theory and pick a particular foliation (preferred "time" variable) of our spacetime. This separation of time and space coordinates is known as 3+1 decomposition of General Relativity, which we set to describe now.

2.1 General relativity in Hamiltonian form

2.1.1 ADM variables

Historically, the first attempt to use canonical quantization for gravity was done by Arnowitt, Deser and Misner and was first published in 1959 [20]. Their method is known as ADM formalism and has played a fundamental role in canonical quantum gravity.

The idea of the method is to assume that our spacetime manifold $(\mathcal{M}, g)$ is globally hyperbolic. In this case, we can foliate our manifold using spatial Cauchy hypersufaces [7] that we will call Σ. We can define the normal to Σ as u^{μ}. The relationship between the metric of our manifold $\mathcal{M}$, $g_{\mu\nu}$, and the metric of the Cauchy surface Σ, which we will call $h_{\mu\nu}$, is given by the first fundamental form:

$$h_{\mu\nu} = g_{\mu\nu} + u_{\mu}u_{\nu}.$$

For each Σ there exists a global parameter t which is a scalar and is constant on the hypersuface, so that $\Sigma = \Sigma(t)$. Now, in order to write the metric components we should introduce coordinates in the manifold that are adapted to our foliation. This coordinates are introduced in the following way [21]: on each hypersurface Σ_t we introduce a coordinate system $x^a = (x^1, x^2, x^3)$. If this coordinate system varies smoothly between hypersurfaces then $x^\mu = (t, x^1, x^2, x^3)$ constitutes a coordinate system in the manifold.

The basis associated to this coordinate system in the tangent space $T_p(\mathcal{M})$ is

$$\partial_\mu = (\partial_t, \partial_a).$$

The vector ∂_t is called the time vector and is tangent to the lines of constant spatial coordinates. On the other hand, the vector ∂_a is tangent to Σ_t, which means that it belongs to $T_p(\Sigma_t)$.

The dual basis associated to ∂_μ is the one-form basis dx^μ, which belongs to the cotangent space of our manifold, $T_p^*(\mathcal{M})$. In particular, the one form $dt = \nabla t$ is dual to ∂_t.

We can now decompose the vector ∂_t in its normal an tangential components with respect to Σ_t [21]:

$$(\partial_t)^\mu = N u^\mu + N^\mu.$$

Here, N is called the lapse function and N^μ is called the shift vector [7, 9, 21]. We'll have that $u_\mu N^\mu = 0$, which means that N^μ is orthogonal to u_μ. This tells us that N^μ belongs to the tangent space of Σ and is three-dimensional, so we can identify it with N^a.

We can then see that the components of u^μ with respect to the basis ∂_μ are

$$u^\mu = \left(\frac{1}{N}, -\frac{N^1}{N}, -\frac{N^2}{N}, -\frac{N^3}{N}\right).$$

While its dual vector components are

$$u_\mu = (-N, 0, 0, 0).$$

The components of the three-metric on the hypersurface Σ_t are h_{ab}. We also have

$$N_a = h_{ab} N^b.$$

We can now compute the components of $g_{\mu\nu}$. The components of the metric g with respect to the coordinates x^μ are given by [21]

$$g = g_{\mu\nu} dx^\mu \otimes dx^\nu.$$

And they can be computed as

$$g_{\mu\nu} = g(\partial_\mu, \partial_\nu).$$

Accordingly, we have

$$g_{00} = g(\partial_t, \partial_t) = \partial_t \cdot \partial_t = -N^2 + N_a N^a.$$

For the $(0, a)$ component, we have

$$g_{oa} = g(\partial_t, \partial_a) = N_a.$$

Finally, we have

$$g_{ab} = g(\partial_a, \partial_b) = h_{ab}.$$

Collecting these results, we can then write the components of the metric tensor as [7, 9, 21]

$$g_{\mu\nu} = \begin{pmatrix} -N^2 + N_a N^a & N_b \\ N_c & h_{ab} \end{pmatrix},$$

whose inverse is

$$g^{\mu\nu} = \frac{1}{N^2} \begin{pmatrix} -1 & N^b \\ N^c & N^2 h^{ab} - N^a N^b \end{pmatrix}.$$

This is the ADM decomposition of the metric.

2.1.2 3+1 decomposition of the action

We begin with the Einstein-Hilbert action [7]

$$S = \frac{1}{16\pi G} \int d^4x \sqrt{-g} R.$$

In the last equation, R is the Ricci scalar and $g = \det(g_{\mu\nu})$. To decompose the action, we would like to write R in terms of the Ricci tensor of our hypersurfaces Σ. To find a relation between the two, we start by introducing the following tensor field:

$$K_{\mu\nu} = h_\mu{}^\rho \nabla_\rho u_\nu.$$

Note that $K_{\mu\nu} n^\mu = K_{\mu\nu} n^\nu = 0$, which means that $K_{\mu\nu}$ is purely spatial and then can be mapped to its spatial counterpart K_{ab}. We can also rewrite $K_{\mu\nu}$ in terms of the Lie derivative [9]:

$$K_{\mu\nu} = \frac{1}{2} \mathcal{L}_{\vec{u}} h_{\mu\nu}.$$

This means that the tensor $K_{\mu\nu}$ tells us how the metric $h_{\mu\nu}$ changes while we move from one hypersurface to another one. $K_{\mu\nu}$ can be used to describe the embedding curvature of Σ into $\mathcal{M}$ at the point p. It is called the extrinsic curvature or second fundamental form [7]. Its trace:

$$K = K_a{}^a = h^{ab} K_{ab}$$

can be interpreted as the expansion of a geodesic congruence orthogonal to Σ. We can write the extrinsic curvature in terms of the shift and the lapse [7]:

$$K_{ab} = \frac{1}{N}\left(\frac{1}{2}\dot{h}_{ab} - \nabla_{(a}N_{b)}\right). \tag{2.1}$$

The relation between the four-dimensional and three-dimensional curvatures is given by the Gauss equation:

$$^{(3)}R_{\mu\nu\lambda}{}^{\rho} = h_\mu{}^{\mu'} h_\nu{}^{\nu'} h_\lambda{}^{\lambda'} h^\rho{}_{\rho'} R_{\mu'\nu'\lambda'}{}^{\rho'} - K_{\mu\lambda}K_\nu{}^\rho + K_{\nu\lambda}K_\mu{}^\rho \tag{2.2}$$

and the generalized Codazzi equation:

$$\nabla_\mu K_{\nu\lambda} - \nabla_\nu K_{\mu\lambda} = h_\mu{}^{\mu'} h_\nu{}^{\nu'} h_\lambda{}^{\lambda'} R_{\mu'\nu'\lambda'}{}^\rho u^\rho. \tag{2.3}$$

Contraction of this last equation with the metric $g^{\mu\lambda}$ gives

$$\nabla_\mu K^\mu{}_\nu - D_\nu K = R_{\rho\lambda} u^\lambda h^\rho{}_\nu. \tag{2.4}$$

Now, let's take a look at the Einstein's equations in vacuum (and without cosmological constant):

$$G_{\mu\nu} = R_{\mu\nu} - \frac{1}{2} g_{\mu\nu} R = 0.$$

For its spacetime component, we find:

$$h^\mu{}_\rho G_{\mu\nu} u^\nu = h^\mu{}_\rho R_{\mu\nu} u^\nu = 0.$$

We can rewrite this equation using (2.4). We obtain:

$$\nabla_b K^b{}_a - \nabla_a K = 0. \tag{2.5}$$

On the other hand, the time-time component of Einstein's equation is

$$G_{\mu\nu} u^\mu u^\nu = R_{\mu\nu} u^\mu u^\nu + \frac{R}{2}.$$

To rewrite this, take equation (2.2) and contract the indices to get

$$^{(3)}R + K_\mu{}^\mu K_\nu{}^\nu - K_{\mu\nu}K^{\mu\nu} = h^{\mu\mu'} h_\nu{}^{\nu'} h_\mu{}^{\lambda'} h^\nu{}_{\rho'} R_{\mu'\nu'\lambda'}{}^{\rho'}$$

The right-hand side of this equation is equal to

$$R + 2R_{\mu\nu}u^\mu u^\nu = 2G_{\mu\nu}u^\mu u^\nu = 0.$$

Then, we obtain

$$^{(3)}R - K_{ab}K^{ab} + K^2 = 0. \tag{2.6}$$

Both equations (2.5) and (2.6) are constraints. However, we can also express equation (2.6) as

$$^{(3)}R - K_{ab}K^{ab} + K^2 = 2R_{\mu\nu}u^\mu u^\nu + R$$

So that we can express the four-dimensional Ricci scalar as

$$R =^{(3)} R - K_{ab}K^{ab} + K^2 - 2R_{\mu\nu}u^\mu u^\nu. \tag{2.7}$$

This is the relationship between the four and three-dimensional Ricci scalars that we were looking for. We can substitute this in the Einstein-Hilbert action, expressing the last term in equation (2.7) using the definition of the Riemann tensor in terms of second covariant derivatives.

After discarding total divergences, rearranging and noting that $\sqrt{-g} = N\sqrt{h}$, we'll get that the Einstein-Hilbert action can be written as [7, 21]

$$S = \frac{1}{16\pi G}\int dtd^3x\ N\sqrt{h}\ (^{(3)}R + K_{ab}K^{ab} - K^2). \tag{2.8}$$

We can cast this action in a slightly different way by defining the DeWitt supermetric:

$$G^{abcd} = \frac{\sqrt{h}}{2}(h^{ac}h^{bd} + h^{ad}h^{bc} - 2h^{ab}h^{cd}),$$

so that the action reads

$$S = \frac{1}{16\pi G}\int dtd^3x\ N(G^{abcd}K_{ab}K_{cd} + \sqrt{h}^{(3)}R). \tag{2.9}$$

Equation (2.9) is called the ADM action [7]. The first term reminds of a classic kinetic term, since the extrinsic curvature has terms that include the time derivative of the metric h_{ab}. This action now has the form we need to apply canonical quantization using the Lagragian

$$\mathcal{L} = \frac{N}{16\pi G}(G^{abcd}K_{ab}K_{cd} + \sqrt{h}^{(3)}R).$$

2.1.3 Defining canonical variables and primary constraints

Once we have the ADM action the next step is to define the canonical variables and their conjugate momenta [7]. Following the procedure described in the last chapter, the canonical variables are h_{ab}, N and N_a. Their conjugate momenta are:

$$\pi^{ab} = \frac{\partial \mathcal{L}}{\partial \dot{h}_{ab}} = \frac{1}{16\pi G} G^{abcd} K_{cd} = \frac{\sqrt{h}}{16\pi G}(K^{ab} - K h^{ab}), \tag{2.10}$$

$$\pi^0 = \frac{\partial \mathcal{L}}{\partial \dot{N}} = 0, \tag{2.11}$$

$$\pi^a = \frac{\partial \mathcal{L}}{\partial \dot{N}_a} = 0. \tag{2.12}$$

One can immediately see that equations (2.11) and (2.12) are to be considered as primary constraints. This means that the following set of primary constraints has to be imposed:

$$\pi^0 \approx 0,$$
$$\pi^a \approx 0.$$

We also have the equal time Poisson bracket relation:

$$\{h_{ab}(x), \pi^{cd}(y)\} = \delta^c_{(a}\delta^d_{b)}\delta(x, y).$$

2.1.4 Dirac Hamiltonian

We are now ready to write the Hamiltonian that corresponds to our theory. Following the procedure discussed in the last chapter, the Hamiltonian is [7, 9]

$$H_D = \int d^3x(\pi^{ab}\dot{h}_{ab} + \pi^0 \dot{N} + \pi^a \dot{N}_a - \mathcal{L}). \tag{2.13}$$

Here, $\dot{N}$ and $\dot{N}_a$ are the Lagrange multipliers corresponding to the primary constraints.

To write the Hamiltonian explicitely, recall equation (2.1) and take the trace of equation (2.10) to express $\dot{h}_{ab}$ in terms of the momenta:

$$\dot{h}_{ab} = \frac{32\pi G}{\sqrt{h}}(\pi_{ab} - \frac{1}{2}\pi h_{ab}) + \nabla_a N_b + \nabla_b N_a.$$

In this case, $\pi = \pi^{ab} h_{ab}$. Substituting this into the Hamiltonian we get:

$$H_D = \int d^3x(N^a\mathcal{H}_a + N\mathcal{H} + \pi^0\dot{N} + \pi^a\dot{N}_a).$$

In this equation we have that

$$\mathcal{H} = 16\pi G\, G_{abcd}\pi^{ab}\pi^{cd} - \frac{\sqrt{h}}{16\pi G}\,{}^{(3)}R, \tag{2.14}$$

$$\mathcal{H}_a = -2\nabla^b\pi_{ab}. \tag{2.15}$$

Since the constraints need to be obeyed at all times, we need to calculate their Poisson bracket with the Hamiltonian and impose that it vanishes:

$$\{\pi^0, H_D\} = -\mathcal{H},$$
$$\{\pi^a, H_D\} = -\mathcal{H}_a.$$

This means that we have to impose [7, 9, 22]

$$\mathcal{H} \approx 0 \qquad\qquad \mathcal{H}_a \approx 0. \tag{2.16}$$

These are called Hamiltonian and diffeomorphism constraints, respectively. It can be proven that they are first class constraints.

Finally, our Hamiltonian is:

$$H_D = \int d^3x(N^a\mathcal{H}_a + N\mathcal{H}). \tag{2.17}$$

Note that the total Hamiltonian is a linear combination of the constraints and then, it is also constrained to vanish weakly.

The diffeomorphism constraint encodes the invariance of the theory under spacetime diffeomorphisms within the three-surfaces Σ, while the Hamiltonian constraint encodes both invariance under time reparametrizations and generates the time evolution of the system [7].

As we discussed in the first chapter, one of the characteristics of first class constraints is that they generate gauge transformations. In the case of General Relativity, the Hamiltonian constraint is first class and it generates the time evolution of our system. Does this mean that the time evolution can be interpreted as a gauge transformation? This is actually the case, since the equation $\mathcal{H} \approx 0$, physically means that evolutions along different foliations are equivalent [4].

Finally, we can count the number of degrees of freedom present in our system. The presence of the constraints means that not all degrees of freedom are physical [13]. To find out how many physical degrees of freedom we have in configuration space, let's begin by noting that the three metric $h_{ab}(x)$ has six degrees of freedom per space point, which means that we begin with $6 \times \infty^3$ degrees of freedom [7].

The diffeomorphism constraint generates coordinate transformations on three-space and the Hamiltonian constraint generates transformations of the time variable [7]. Together, they correspond to four variables per space point ($4 \times \infty^3$) that must be subtracted from our initial number of degrees of freedom.

After subtracting, we are left with $2 \times \infty^3$ remaining degrees of freedom that correspond to the two polarizations of the graviton [4].

2.2 Canonical quantization

After formulating General Relativity in the Hamiltonian formalism, we are ready to perform canonical quantization. The idea is to implement Dirac's programme to get a quantum theory of gravity. However, General Relativity has a special feature: the Hamiltonian is a combination of the constraints, which means that it vanishes weakly. The fact that the dynamics of the system is completely described by the constraints will have important consequences, one of them being the problem of time [6].

We begin by promoting the configuration variables and their conjugate momenta to operators. As we saw before, the fundamental variables are the three-metric h_{ab} and its conjugate momenta π^{ab}. We have:

$$h_{ab} \longrightarrow \hat{h}_{ab}, \qquad\qquad \pi^{ab} \longrightarrow \hat{\pi}^{ab}.$$

The classical Poisson bracket is replaced by the commutator:

$$[\hat{h}_{ab}(\vec{x}), \hat{\pi}^{cd}(\vec{y})] = i\hbar\delta^c_{(a}\delta^d_{b)}\delta(\vec{x}, \vec{y}).$$

Now we should construct a representation space for the dynamical variables, on which they act as operators. We will define an element of the Hilbert space as functionals $\Psi[h_{ab}]$ of the canonical variables and we'll implement

$$\begin{aligned}\hat{h}_{ab}(\vec{x})\Psi[h_{ab}(\vec{x})] &= h_{ab}(\vec{x})\Psi[h_{ab}(\vec{x})],\\ \hat{\pi}(\vec{x})^{cd}\Psi[h_{ab}(\vec{x})] &= -i\hbar\frac{\delta}{\delta h_{cd}(\vec{x})}\Psi[h_{ab}(\vec{x})].\end{aligned}$$

The next step is the implementation of the constraints. Choosing operators to act on the right, the diffeomorphism constraint is:

$$\hat{\mathcal{H}}_a\Psi = 2i\hbar\nabla^a\frac{\delta}{\delta h^{ab}}\Psi = 0. \tag{2.18}$$

This condition is satisfied if Ψ is invariant under coordinate transformations in the hypersurface Σ [7]. This is in agreement with the classical interpretation of the diffeomorphism constraint as the generator of diffeomorphisms on Σ.

The quantum dynamics is governed by the Hamiltonian constraint. With derivative operators acting to the right of the DeWitt metric, it reads [7, 9]:

$$\hat{\mathcal{H}}\Psi = \left[16\pi G\hbar^2 G_{abcd}\frac{\delta^2}{\delta h_{ab}\delta h_{cd}} + \frac{\sqrt{h}}{16\pi G}\ {}^{(3)}R\right]\Psi = 0. \tag{2.19}$$

Only solutions to equations (2.18) and (2.19) can be considered physical states. Equation (2.19) is known as the **Wheeler-DeWitt equation** [7, 9, 6, 4] and is the starting point of many approaches to quantum cosmology and quantum gravity.

In chapter 2, we mentioned that observables are characterized by having vanishing Poisson bracket with the constraints. To translate this to the quantum theory, for an operator corresponding to a classical observable that satisfies $\{O, \mathcal{H}_\mu\} \approx 0$ where $\mathcal{H}_\mu$ are our constraints, we expect that the following relation holds [7]:

$$[\hat{O}, \hat{\mathcal{H}}_\mu]\Psi = 0.$$

The last step of the quantization process concerns the Hilbert space. What is the Hilbert space that corresponds to our theory? Is it the space of solutions to equations (2.18) and (2.19)? One would expect that this space is still too big, since there are still some conditions that should be imposed in our wave functions, like normalizability [23]. In general, it is unclear which one should be taken as the Hilbert space of the theory and there is no easy way around this.

This in principle concludes the canonical quantization of General Relativity. Let us, however, make some more comments about the interpretation of equation (2.19).

We have argued that equation (2.19) governs the quantum dynamics of the system. However, we can see that the right hand side of this equation is equal to zero. What does this mean for the evolution of the wave equation Ψ? To make an analogy, let's remember the Schrödinger equation. The Schrödinger equation tells us that the Hamiltonian acting on the wave equation gives us its time evolution. The Hamiltonian in this case also acts as the generator of time evolution.

On the other hand, we have equation (2.19). This equation tells us that the Hamiltonian constraint acting on the wave function is equal to zero. Since the Hamiltonian constraint is the generator of time evolution, the Wheeler-DeWitt equation seems to tell us that there is no time evolution for the wave function Ψ. In other words, Ψ seems to be "frozen" [4] and time is missing in our formalism. This apparent absence of time in our theory has to be accounted for somehow. This is **the problem of time** [4, 6].

This was to be somehow expected, since one of the main ideas of General Relativity is that the laws of physics should be independent of the coordinates we use [3]. However, time is usually regarded as a coordinate in our manifold, so we should expect that it plays no fundamental role in our theory [6].

But if time is supposed to play no fundamental role in our theories, how does change arise in our formalism? We'll study different possibilities to answer this question in the following chapters in the context of minisuperspaces. But before, let us discuss the problem of time in detail.

Chapter 3

The problem of time

As we mentioned at the end of the last chapter, the Wheeler-DeWitt equation doesn't contain evolution in time, making our wavefunction to appear "frozen". This raises several questions about the interpretation of the concept of time in quantum gravity [4, 6]. In particular, some of the most relevant questions that require an answer are the following: how can we reintroduce the concept of time and evolution in a quantum theory of gravity? Is time a fundamental concept or is it phenomenological? If time is phenomenological, how reliable is the rest of quantum mechanics in the regimes where the concept of time is not applicable?

The key to understanding where the problem of time comes from is to think about the different roles that time plays in quantum mechanics and General Relativity [2]. On one hand, we have quantum mechanics. The concept of time used in conventional quantum mechanics is that of Newtonian physics [2], in which time is a fixed structure external to the system. This is reflected in the formalism of quantum mechanics in different ways:

- Time is not represented by an operator but is treated as a background parameter used to mark the evolution of the system [24].
- Since time is an external parameter to the system, there is a difficulty to describe a truly closed system in quantum mechanics [25]. We always need to define the quantum system under study and the observer, who is the one who takes care of making measurements and keeps track of time. The observer is usually kept classical.
- The idea of events that happen at a particular time plays a fundamental role in quantum mechanics [4]. For example, measurements are made at a particular time in the Copenhagen interpretation, an observable is an object that can be measured at a fixed time, the scalar product on the Hilbert Space is required to be conserved under time evolution and complete set of observables are required to commute at a fixed time value.

On the other hand we have General Relativity, which is invariant under diffeomorphisms. This means that equations transform covariantly under changes of spacetime coordinates and physical quantities should be independent of our choice of coordinates [3, 7, 6]. However, time is usually regarded as one of the coordinates in our manifold. So, we should expect that it plays no fundamental role in our theories. But then again, if time is supposed to play no role in our theories how does change arise?

These difficulties that the invariance under diffeomorphisms poses are not present in the classical theory. This is because once the field equations are solved we can use the metric to give meaning to concepts like causality and spacelike separation of hypersurfaces [4]. However, in the quantum theory the metric will be subjected in some sense to quantum fluctuations, and since the concepts of causality and spacelike separation depend on the metric, they seem to be state dependent. Does this mean that the concept of time is also state dependent?

The problem of time is also related to some important conceptual problems that must be addressed in order to get a coherent theory of quantum gravity [4]. Some examples of these issues are: the concept of probability and whether it is conserved, the extent to which spacetime is a meaningful concept or should be substituted in the quantum theory, the extent to which the classical geometrical concepts of General Relativity can be maintained in the quantum theory and the question of the interpretation of quantum mechanics and in particular, the status of the Copenhagen interpretation.

Over the years, there have been mainly three ways to approach the problem of time, which we now discuss.

3.1 Approaches to the problem of time

Following Kuchar [6], currently, there are mainly three ways to treat the problem of time in quantum gravity, most of the approaches have been developed in the context of quantum cosmology, specifically for minisuperspaces. We will briefly review them and list some of the most relevant works addressing each of them and the issues that each approach presents.

3.1.1 Internal Time Framework

This approach considers that time is hidden among the canonical variables and it should be identified before quantization. The main equation in this approach is the Schrödinger equation instead of the Wheeler-DeWitt equation.

These approaches, however, suffer from the multiple choice problem. The principal idea behind this problem is that the Schrödinger equations defined for different time parameters lead to different quantum theories and there is no easy criteria to choose one over other. Examples of this approach can be found in [26], [22], [12].

The Internal Time Framework approach can be further subdivided into the following specific approaches:

Internal Schrödinger interpretation

Time and space coordinates are identified as functions of the gravitational canonical variables and are separated from the dynamical degrees of freedom by a gauge transformation. The constraints are then solved for the conjugate momenta to this variables and the remaining variables are then quantized. Quantization gives rise to a Schrödinger equation for the physical states.

Matter clocks and reference fluids

In this approach, matter variables coupled to the geometry are used to label events. It is an extension of the the internal Schrödinger interpretation.

Unimodular gravity

In this approach the cosmological constant is considered a dynamical variable and a cosmological time is defined as its canonical conjugate. The constraints yield the Schrödinger equation with respect to this time. It is a particular case of a reference fluid. Examples of this approach can be found in [27, 28, 29]

3.1.2 Wheeler-DeWitt Framework

In this approach time is identified after quantization. Constrainst are imposed at a quantum level to yield the Wheeler-DeWitt equation and one tries to give a dynamical interpretation to its solutions.

This approach suffers from the so-called Hilbert Space Problem. To understand what this problem means, it is enough to realize that, unlike the Schrödinger equation, the Wheeler-DeWitt equation doesn't provide us with either a conserved inner product or a way to construct observables at a given time. In other words, being a second order differential equation, the Wheeler-DeWitt equation presents problems when one tries to build a Hilbert Space from the space of its solutions. Examples of this approach can be found in [30], [19].

This approach can be further subdivided in three categories:

The Klein-Gordon interpretation

The Wheeler-DeWitt equation is considered an infinite dimensional analogue of the Klein-Gordon equation for a relativistic particle. The probabilistic interpretation is based on the Klein-Gordon inner product, which is expected to be positive on some subspace of solutions of the Wheeler-DeWitt equation.

Third quantization

The problems arising from the fact that the Klein-Gordon inner product is indefinite are addressed by suggesting that the solutions to the Wheeler-DeWitt equation are to be turned into operators. This is analogous to the second quantization performed in quantum field theory. Examples on this approach can be found in [31, 32, 33].

The semiclassical interpretation

In this approach, time emerges and is a meaningful concept just in the semiclassical limit of the quantum theory of gravity based in the Wheeler-DeWitt equation. Writing the wavefunction using a WKB approximation, the Wheeler-DeWitt equation is approximated by the Schrödinger equation and the time variable is extracted directly from the wavefunction.

3.1.3 Quantum Gravity Without Time

These approaches are based mostly in the Wheeler-DeWitt equation and they support the idea that time is not needed to interpret either quantum gravity or quantum mechanics [23]. Time, however, appears in particular situations. For an example of a proposal of a formulation of quantum mechanics that doesn't rely on a time parameter see [34].

The approaches to quantum gravity that don't rely in the identification of a time parameter can be further classified into four more categories, which we will proceed to describe briefly.

Naïve Schrödinger interpretation

In this approach it is considered that the square of solutions to the Wheeler-DeWitt equation are to be interpreted as the probability of finding a hypersurface with the metric $\mathbf{g}$. This interpretation was proposed by Hawking in [35].

However, this interpretation has the problem that it lacks dynamics, in the sense that is not capable to give an answer to dynamical questions that we can usually ask in the usual quantum theory [6].

The conditional probability interpretation

It is an attempt to include dynamics into the Naïve Schrödinger interpretation. It was developed by Page and Wootters. See [25].

Sum-Over-Histories Interpretation

These approaches rely on the use of the path integral formalism to give an interpretation to quantum gravity. The premise is that the path integral formalism can be used to interpret quantum systems that don't have an automatic notion of time and Hilbert Space. This approach was mainly developed by Hartle, see [36].

Frozen Time Formalism and Evolving Constants of the Motion

These approaches try to answer the question of what is an observable in General Relativity. In general, in a gauge theory an observable is a quantity that is left unchanged by gauge transformations. Since in the case of general relativity the Hamiltonian is a generator of gauge transformation, we are led to the conclusion that the observables, which are defined to be gauge invariant, must be constants of the motion [37].

But if the observables are constants of the motion, then it would seem that the Universe can't change. This was called The Frozen Time Formalism. This formalism can't explain the evolution of the universe.

However, Rovelli reinterpreted this formalism in a way that allows to describe evolution by introducing the concept of evolving constants of motion [38] [39]. A recent work using this formalism can be found in [17].

3.2 The different facets of the problem of time

In all the approaches to the problem of time discussed previously a series of technical problems are expected to appear [2]. Some of the most important ones are the following [4, 6]:

- **The ultraviolet divergence problem:** Quantum gravity is non-renormalisable in perturbation theory. This suggest that the operator analogues of some complicated classical expressions that involve fields defined at the same spacetime point are ill-defined. Since the internal time and Wheeler-DeWitt frameworks involve expressions of this kind, we could ask whether this approaches are valid.

- **The operator-ordering problem:** When promoting the constraints to operators, we find complicated operator ordering difficulties. This is connected to the ultraviolet divergence problem.

- **The global time problem:** The extraction of the dynamics of a system can pose problems even at the classical level. In particular, to extract the dynamics we must separate time from the dynamical variables. This may be globally impossible in the sense that there may not exist a canonical transformation that allows us to do this separation. The global problem of time is purely classical.

- **The multiple choice problem:** The Schrödinger equation that we find after choosing a particular time variable may give a different quantum theory than the Schrödinger equation based on another choice of internal time. Which one is correct? The multiple choice problem is different from the global problem of time, since in the first case we have many possible time variables and no criteria to choose one in particular, while in the second case we have no options at all.

- **The Hilbert space problem:** The advantage of the internal time framework is that we end up with a Schrödinger equation. As we know, the Schrödinger equation automatically gives us an inner product that is conserved in the selected time variable. This is not the case for the Wheeler-DeWitt equation, which is a second-order functional differential equations that presents problems when we try to construct a positive definite inner product in its space of solutions.

- **The spatial metric reconstruction problem:** The separation of variables into physical and non-physical can be inverted and the metric can be expressed in terms of these variables. The spatial metric reconstruction problem deals with the question of whether something like this can be done also in the quantum theory. This problem is related to the question if the classical geometric properties are preserved or not in the quantum theory.

- **The spacetime problem:** It is necessary that the chosen time and space coordinates, viewed as functions on the manifold, be scalar fields and don't depend on any foliation. However, the objects used in the canonical approach to quantum gravity are functionals of the canonical variables and they might not satisfy this condition. We should find functionals that have this property or, in case it is not possible to do so, we should understand how to handle the situation.

- **The problem of functional evolution:** In some cases the evolution of a state from an initial hypersurface to a final hypersurface can depend on the foliation that connects them. This means that when we start with some initial state on the initial hypersurface and evolve it to the final hypersurface along two different routes the two final states are different.

These problems usually appear in the internal time framework and the Wheeler-DeWitt framework. They are less relevant in the quantum gravity without time framework, since time in this approach only plays a secondary role [4]. However, still in this framework analogues of these problems keep appearing, adding extra difficulty to the approach.

Since quantum gravity is a little understood system, it is common to try to study it in the context of simpler models that share relevant features with the full theory, including the problem of time. In particular, minisuperspace models have played a fundamental role both in quantum cosmology and in the study of quantum gravity [4]. In the present thesis work, we are going to study the problem of time in the case of a flat FLRW spacetime coupled to a scalar field. In order to do this, we have to apply what we have already discussed in the last chapters to this cosmological model. Performing the canonical quantization of this system is the subject of the next chapter.

Chapter 4

Quantum minisuperspace

It is very hard to deal with the full formalism of canonical quantum gravity since its configuration space is infinite dimensional. It is because of this that attempts to study quantum gravity are usually made on simpler models that share relevant features with the full formalism [6].

In particular, quantum cosmology plays an important role in the study of quantum gravity because cosmological models are simple examples to which the ideas of a quantum theory of gravity can be applied. Also, it is expected that quantum gravity effects played a fundamental role in the inflationary phase of the universe, so that it is possible that they have left a print in the cosmic microwave background [4].

Most advances in quantum cosmology have been done in the context of a simple class of models call minisuperspaces [6]. These models are characterized by the imposition of symmetries that freeze infinitely many degrees of freedom, as a consequence minisuperspaces have a finite dimensional configuration space.

Examples of minisuperspaces are the well-known Friedmann-Lemaître-Robertson-Walker (FLRW) cosmologies, the Bianchi space-times [40], and the Kantowski-Sachs universes [41].

These models share relevant features with the full theory of quantum gravity and in particular, the problem of time is present in all of them [22]. Studying the problem of time in this simpler models can give us insight about how to solve it in the context of the full theory.

In this chapter we will study the Hamiltonian formulation and the quantization of the flat FLRW cosmology coupled to a scalar field. The results of this chapter will be used later to study different possibilities to include time in this particular model.

4.1 Flat FLRW spacetime minimally coupled to a scalar field

We start from the Einstein-Hilbert action minimally coupled to a massless scalar field [7]:

$$S = \int d^4x\sqrt{-g}\left(\frac{R}{8\pi G} - \partial_\mu\phi\partial^\mu\phi\right).$$

We want to write the theory in Hamiltonian form, so that we can perform canonical quantization. In order to do this, we'll apply the 3+1 decomposition discussed in Chapter 2. Using the foliation in Cauchy hypersurfaces, the FLRW metric reads:

$$ds^2 = -(N^2 - N_aN^a)dt^2 + 2N_a dx^a dt + a^2(t)(dx^2 + dy^2 + dz^2).$$

Here, N is the lapse function, N_a is the shift vector and $a(t)$ is the scale factor. In this case the shift vector can be set to zero and the metric is just

$$ds^2 = -N^2dt^2 + a^2(t)(dx^2 + dy^2 + dz^2).$$

Using this metric, we can calculate the Ricci scalar

$$R = \frac{6}{N^2}\left(\frac{\ddot{a}}{a} - \frac{\dot{a}}{a}\frac{\dot{N}}{N} + \frac{\dot{a}^2}{a^2}\right).$$

In the last equation, a dot implies derivative with respect to time. Substituting the Ricci scalar in the action, we get:

$$S = \int dtNa^3\left[\frac{6}{8\pi GN}\left(\frac{\ddot{a}}{\dot{a}} - \frac{\dot{a}}{a}\frac{\dot{N}}{N} + \frac{\dot{a}^2}{\dot{a}^2}\right) + \frac{\dot{\phi}^2}{2N^2}\right].$$

We can rewrite this action in a simpler way by adding the boundary term $-6\frac{d}{dt}\left(\frac{a^2\dot{a}}{N}\right)$. We will also rescale the Planck mass, that we will call M and rearrange to get

$$S = \int dt\left(-\frac{M^2a\dot{a}^2}{2N} + \frac{a^3\dot{\phi}^2}{2N}\right). \tag{4.1}$$

So that the Lagrangian of this theory is [22]:

$$\mathcal{L} = -\frac{M^2a\dot{a}^2}{2N} + \frac{a^3\dot{\phi}^2}{2N}. \tag{4.2}$$

Before moving to find the Hamiltonian of this theory and quantize it, let us study the classical Lagrangian dynamics of the system. We can perform variations in the action (4.1) with respect to $a(t)$, N and ϕ to obtain the equations of motion:

$$\delta_a S = 0 \longrightarrow \frac{\ddot{a}}{a} + \frac{3}{2}\frac{\dot{a}^2}{a^2} - \frac{\dot{a}\dot{N}}{aN} = \frac{3}{2}\frac{\dot{\phi}^2}{M^2}, \tag{4.3}$$

$$\delta_\phi S = 0 \longrightarrow p_\phi = \frac{a^3\dot{\phi}}{N} = \text{constant}, \tag{4.4}$$

$$\delta_N S = 0 \longrightarrow \frac{M^2 a\dot{a}^2}{N^2} - \frac{a^3\dot{\phi}^2}{N^2} = 0. \tag{4.5}$$

We can write equation (4.5) in terms of p_ϕ to find

$$\frac{M^2 a\dot{a}^2}{N^2} = \frac{p_\phi^2}{a^3}. \tag{4.6}$$

To solve the equations of motion we need to choose N. This is equivalent to picking a Gauge. The simplest choice is to set $N = 1$ that corresponds to the proper or synchronous time. Setting $N = 1$ we can solve (4.6) to get

$$a^3(t) = a_0^3 \pm \frac{3|p_\phi|}{M} t,$$

Here, $a_0 = a(0)$ and the $\pm$ sign gives an expanding or contracting universe.

4.2 Hamiltonian dynamics

To calculate the Hamiltonian of our system, it is convenient to parametrize the scale factor as [22]

$$a(t) = e^{\alpha(t)}.$$

Using this parametrization the Lagrangian reads

$$\mathcal{L} = -\frac{M^2\dot{\alpha}^2 e^{3\alpha}}{2N} + \frac{\dot{\phi}^2 e^{3\alpha}}{2N}. \tag{4.7}$$

Using this Lagrangian we can calculate the conjugate momenta to the variables N,α and ϕ:

$$p_N = 0, \qquad p_\alpha = -\frac{M^2\dot{\alpha}e^{3\alpha}}{N}, \qquad p_\phi = \frac{\dot{\phi}e^{3\alpha}}{N}.$$

We can then write the Hamiltonian

$$H = p_N \dot{N} + p_\alpha \dot{\alpha} + p_\phi \dot{\phi} - \mathcal{L}.$$

This gives

$$H_D = N\left(-\frac{p_\alpha^2 e^{-3\alpha}}{2M^2} + \frac{p_\phi^2}{2} e^{-3\alpha}\right) = N\mathcal{H}.$$

Since $p_N = 0$ is a primary constraint, we have to make sure that it holds at all times. This yields the Hamiltonian constraint:

$$\{p_N, H_D\} = \mathcal{H} \approx 0.$$

This tells us that H_D is constrained to vanish weakly. We can find the equations of motion by calculating the Poisson bracket:

$$\begin{aligned}
\dot{\phi} &= \{\phi, H_D\} = Ne^{-3\alpha} p_\phi, \\
\dot{p_\phi} &= \{p_\phi, H_D\} = 0, \\
\dot{\alpha} &= \{\alpha, H_D\} = -\frac{Ne^{-3\alpha} p_\alpha}{M^2}, \\
\dot{p_\alpha} &= \{p_\alpha, H_D\} = -\frac{\partial H_D}{\partial \alpha} = 3H_D \approx 0.
\end{aligned}$$

We can see that p_ϕ and p_α are conserved.

4.3 Quantization

We now proceed to quantize the system. In order to do that, we must promote the variable to operators and choose a representation. On promoting our canonical variables to operators, and choosing the simplest operator ordering, we obtain the Hamiltonian operator:

$$\hat{\mathcal{H}} = e^{-3\hat{\alpha}}\left(-\frac{\hat{p}_\alpha^2}{2M^2} + \frac{\hat{p}_\phi^2}{2}\right).$$

We obtain then the Wheeler-DeWitt equation:

$$\hat{\mathcal{H}} \left|\Psi\right\rangle = 0.$$

Since p_ϕ is conserved it is convenient to work in a mixed representation [22] so that our operators will act on the wave functions $\Psi(\alpha, p_\phi)$ in the following way

$$\hat{p}_\alpha \Psi(\alpha, p_\phi) = -i\frac{\partial}{\partial \alpha}\Psi(\alpha, p_\phi), \qquad \hat{p}_\phi \Psi(\alpha, p_\phi) = p_\phi \Psi(\alpha, p_\phi).$$

Using this representation the Hamiltonian operator reads

$$\hat{\mathcal{H}} = \frac{e^{-3\alpha}}{2M^2}\left(\frac{\partial^2}{\partial \alpha^2} + M^2 p_\phi^2\right)$$

So that the Wheeler-deWitt equation reads [22]

$$\left(\frac{\partial^2}{\partial \alpha^2} + M^2 p_\phi^2\right)\Psi(\alpha, p_\phi) = 0. \tag{4.8}$$

As we expected, in equation (4.8) time is not present, indicating that $\Psi(\alpha, p_\phi)$ seems to be frozen. How can we introduce time in this model? In the following chapters we will discuss different ways to reintroduce time in this system in order to obtain an evolving cosmology.

Chapter 5

Time before quantization

Up to now we have seen that after performing the $3+1$ decomposition of the Einstein-Hilbert action, defining canonical variables and identifying the primary constraints, we can write the Hamiltonian [7, 9]

$$H_D = \int d^3x (N^a \mathcal{H}_a + N\mathcal{H}).$$

Here, N and N_a are called the lapse function and the shift vector and $\mathcal{H}$, $\mathcal{H}_\alpha$ are called the Hamiltonian and diffeomorphism constraint, correspondingly. We have also seen that the super Hamiltonian and the super momentum are constrained to vanish weakly, which means that also the Hamiltonian will vanish weakly. This have the consequence that our quantum states will appear to be "frozen" [7, 6, 4].

Upon quantization both the super Hamiltonian and the super momentum are turned into operators that act on our quantum states [14]. The quantum dynamics is governed by the Hamiltonian constraint:

$$\hat{\mathcal{H}} \left|\Psi\right\rangle = 0.$$

This equation is known as the Wheeler-DeWitt equation. The absence of time reflects one of the main features of General Relativity: time and space are treated on equal footing, meaning that time is also dynamic and the time evolution of the gravitational field is locally just a gauge Transformation [12]. We should expect this, because the reparametrizations of the time variable belong to the gauge group of the theory, which in the case of General Relativity is the group of diffeomorphism on the spacetime meanifold

Is there any way around this? To answer this question we should take a look carefully at the formalism of quantum mechanics. In our discussion in the Chapter 3, we mentioned that one of the hearts of the problem of time is that in quantum mechanics we never describe systems that are truly isolated. When describing a quantum mechanical system we have to define the quantum system and the observer, which is kept classical and takes care of doing measures and keeping track of time. But cosmological systems are truly closed systems, all the information in the universe is contained in the system and there is not outside observer that can keep track of time [4].

With this is mind, a possible way to solve the problem of time could be to choose our dynamical variables in such a way that one degree of freedom is kept classical, so that it can be used as a clock. Let's first describe the general method, developed in [12] and then explore some its consequences making use of a simple cosmological model.

5.1 Choosing dynamical variables

Suppose we are studying some dynamical system that we would like to quantize. However, this system happens to have a constrained Hamiltonian of the type $H_\tau(q,p) = 0$, where τ is a time parameter in terms of which our problem was formulated and (q,p) actually mean $\{q^a, p_a\}$ with $a = 1, ..., n$.

We are going to look for a canonical transformation that takes us from the variables $\{q^a\}$ and $\{p_a\}$ to new variables $\{Q^\mu\}$ and $\{P_\mu\}$ with $\mu = 0, ..., n-1$. We are going to choose our new variables in such a way that

$$\frac{dQ^0}{d\tau} = \{Q^0, H_\tau\} = 1. \tag{5.1}$$

Here, $\{\cdot,\cdot\}$ denote the Poisson bracket. We can see that equation (5.1) implies that we can write our Hamiltonian, H_τ as

$$H_\tau = P_0 + H(Q^0 ... Q^{n-1}, P_1 ... P_{n-1}). \tag{5.2}$$

In this equation, H is called the effective or physical Hamiltonian [12]. As we can see, H doesn't depend on P_0, so when we perform canonical quantization by replacing $P_0 \to -i\hbar\frac{\partial}{\partial Q^0}$, the equations $H_\tau = 0$ will become a time dependent schrödinger equation for the new time Q^0 and the $n-1$ variables $Q^1, ..., Q^{n-1}$.

Then, our main task is to find a suitable function $Q^0(q,p)$ to serve as a clock. Remembering what we said before, this function should have Poisson bracket with the Hamiltonian equal to one. In other words, we need a canonical transformation such that $Q^0 = f(q,p)$. So, from equation (5.1) we can see that

$$\{f(q,p), H_\tau\} = 1 = \frac{dQ^0}{d\tau}.$$

There is an important subtlety here. We are claiming that we are going to look for a function of the phase space variables whose Poisson bracket with the Hamiltonian are equal to 1. But where should the Poisson bracket be equal to one? In the whole phase space? Or only in the constrained surface? In his paper [12], Peres argues that consistency of the method requires the Poisson bracket to be equal to one in the whole phase space. However, it is not clear if this condition is necessary and sufficient. In fact, we will later see two examples, one in which the Poisson bracket is equal to one only on the constrained surface and other one in which it is one in the whole phase space. We will find interesting features in both cases.

Going back to our problem, we need to find a canonical transformation that allows us to write the Hamiltonian as $H_\tau = P_0 + H$. We can do this by solving a first order partial differential equation. The easiest way to do it is to use a generating function of type F_1, that we will call $S(q, Q)$.

Making use of this generating function, we would have

$$p_k = \frac{\partial S}{\partial q^k} \qquad\qquad P_\mu = -\frac{\partial S}{\partial Q^\mu}. \tag{5.3}$$

Then, substituting equation (5.3) in $Q^0 = f(q, p)$ we get that to obtain $S(q, Q)$ explicitly we have to solve

$$Q^0 = f\left(q, \frac{\partial S(q, Q)}{\partial q}\right). \tag{5.4}$$

The Q^μ with $\mu > 0$ are unspecified integration constants in the solution of (5.4) [12].

Once we have solved our differential equation, we can get $P_\mu(q, Q)$ and $p(q, Q)$ using equation (5.3). Having $P_\mu(q, Q)$, we can invert it to get $q(Q, P)$, which we can substitute into $p(q, Q)$ to get $p(Q, P)$. Finally, we have to substitute all these results into H_τ in order to write it in the form given by equation (5.2).

Now we can apply canonical quantization to (5.2) in the usual way, making $P_0 \to -i\hbar\frac{\partial}{\partial t}$ where we have replaced Q^0 by a new variable t. Note that t is going to be a function of the phase space coordinates. This means that this is a dynamical time, and not a gauge dependent coordinate-time [12]. Finally, our wave function $\Psi(q, Q^0)$ must be normalized according to

$$\int |\Psi(q, Q^0)|^2 dq = 1,$$

Without integration in dQ^0. This is because Q^0 will play the role of the time parameter.

This concludes the discussion of the method to be employed. Now, we will proceed to apply this method in the case of a spatially flat FLRW universe coupled to a scalar field using the results we have obtained in Chapter 4. We will do it in three different ways, and then try to compare the results.

5.2 Finding the time function by solving the equations of motion

We will begin by considering the metric of a spatially flat FLRW universe coupled to a scalar field. In chapter 4 we saw that a Lagrangian for this theory is (4.2):

$$\mathcal{L} = -\frac{M^2 a\dot{a}^2}{2N} + \frac{a^3\dot{\phi}^2}{2N}. \tag{5.5}$$

We can easily find the conjugate momenta and the equations of motion using this Lagrangian. The results, as we already saw, are:

$$p_N = \frac{\partial L}{\partial \dot{N}} = 0 \qquad \dot{p}_N = \frac{\partial L}{\partial N} = -\frac{1}{2N^2}(a^3\dot{\phi}^2 - M^2 a\dot{a}^2) = 0, \tag{5.6}$$

$$p_\phi = \frac{\partial L}{\partial \dot{\phi}} = \frac{a^3\dot{\phi}}{N} \qquad \dot{p}_\phi = \frac{\partial L}{\partial \phi} = 0, \tag{5.7}$$

$$p_a = \frac{\partial L}{\partial \dot{a}} = -\frac{M^2 a\dot{a}}{N} \qquad \dot{p}_a = \frac{\partial L}{\partial a} = \frac{1}{2N}(3a^2\dot{\phi}^2 - M^2\dot{a}^2). \tag{5.8}$$

Now, to make the following calculations easier we are going to introduce a new variable τ that we'll define as $d\tau = Ndt$. Substituting this in our Lagrangian (5.5), we'll get a new Lagrangian $\mathcal{L}_\tau d\tau = \mathcal{L}dt$. So, our action will remain invariant. Another convenient change of variables is to introduce $v(t) = a^3(t)$. Making this changes our new Lagrangian will be given by:

$$\mathcal{L}_\tau = \frac{v}{2}\left(\frac{d\phi}{d\tau}\right)^2 - \frac{M^2}{18v}\left(\frac{dv}{d\tau}\right)^2. \tag{5.9}$$

Using this Lagrangian we can calculate the conjugate momenta:

$$p_\phi = v\frac{d\phi}{d\tau}, \tag{5.10}$$

$$p_v = -\frac{M^2}{9v}\frac{dv}{d\tau}. \tag{5.11}$$

We can then write the Hamiltonian:

$$H_\tau = p_\phi\dot{\phi} + p_v\dot{v}_v - L_\tau.$$

Substituting (5.10) and (5.11) in the last equation we get:

$$H_\tau = \frac{1}{2v}p_\phi^2 - \frac{9v}{2M^2}p_v^2. \tag{5.12}$$

Note that (5.9) and (5.12) vanish weakly because of the constraint (5.6). Also, we have gotten rid of the variable $N(t)$. However, we can't get rid of the constraint associated to this variable, equation (5.6).

The equations of motion, as we already know, are

$$\dot{p}_\phi = 0.$$

$$\dot{p}_v = \frac{1}{2v^2}p_\phi^2 + \frac{9}{2M^2}p_v^2.$$

Now, we'll devote ourselves to our main task: finding a time function $Q^0 = f(v, p_v, p_\phi)$ such that $\frac{dQ^0}{d\tau} = \{f(v, p_v, p_\phi), H_\tau\} = 1$. In order to do this, we'll solve the equations of motion. Begin by substituting equation (5.11) into the Hamiltonian (5.12) to get:

$$\frac{1}{2}\left(\frac{dv}{d\tau}\right)^2 + \frac{9v}{M^2}H_\tau = \frac{9}{2M^2}p_\phi^2.$$

The solution of this differential equation is

$$v(\tau) = -\frac{9}{2}\frac{H_\tau}{M^2}\tau^2 \pm \frac{3p_\phi}{M}\tau. \tag{5.13}$$

Here, the integration constant is set so that $v(0) = 0$. By definition $v \geq 0$, so the $\pm$ sign has to be equal to the sign of $p_\phi\tau$. We won't use the constraint $H_\tau = 0$ here, because we want to get a time function that is valid in all the phase space and not only in the constraint surface. Our goal is to get $\tau = f(v, p_v, p_\phi)$. To get it, take (5.13) and derive it with respect to τ to get

$$\frac{dv}{d\tau} = -\frac{9}{M^2}H_\tau\tau \pm \frac{3p_\phi}{M}. \tag{5.14}$$

From equation (5.11) we have

$$vp_v = -\frac{M^2}{9}\frac{dv}{d\tau}. \tag{5.15}$$

Multiply equation (5.14) by $-\frac{M^2}{9}$ and substitute in equation 5.15 to get

$$vp_v = H_\tau\tau \mp \frac{Mp_\phi}{3}. \tag{5.16}$$

Substitute this last equation on (5.13) to get

$$-\frac{2M^2}{9}v = \tau\left(vp_v \mp \frac{Mp_\phi}{3}\right).$$

So that our final result is

$$\tau = f(v, p_v, p_\phi) = \frac{v}{-\frac{9}{2M^2} v p_v \pm \frac{3p_\phi}{2M}}. \tag{5.17}$$

It's not hard to verify that $\{f(v, p_v, p_\phi), H_\tau\} = 1$. Let's see it quickly:

$$\{f(v, p_v, p_\phi), H_\tau\} = \frac{\partial f}{\partial v}\frac{\partial H_\tau}{\partial p_v} = \frac{\left(-\frac{9}{2M^2} v p_v \pm \frac{3p_\phi}{2M}\right)^2}{\left(-\frac{9}{2M^2} v p_v \pm \frac{3p_\phi}{2M}\right)^2} = 1.$$

Now that we have found $\tau = f(v, p_v, p_\phi)$ the next step is to find the generator of the transformation from the coordinates (v, ϕ, p_v, p_ϕ) to the new coordinates that include (Q^0, P^0). Remember that we saw that

$$Q^0 = f\left(q, \frac{\partial S}{\partial q}(q, Q)\right).$$

Using this we can write

$$Q^0 = \frac{v}{-\frac{9}{2M^2} v \left(\frac{\partial S}{\partial v}\right) \pm \frac{3}{2M}\left(\frac{\partial S}{\partial \phi}\right)}, \tag{5.18}$$

Here, we have $S = S(v, \phi, Q^0, Q^1)$. Now, we should solve (5.18). One way to solve it is to use separation of variables:

$$S = \phi Q^1 + S'(v, Q^0, Q^1). \tag{5.19}$$

In this case we'll have $Q^1 = p_\phi$. Substituting this in (5.18) and rearranging we get

$$\frac{\partial S'}{\partial v} = -\frac{2M^2}{9}\frac{1}{Q^0} \pm \frac{M}{3}\frac{Q^1}{v}. \tag{5.20}$$

The solution to this differential equation seems to be:

$$S' = \left(-\frac{2M^2}{9}\frac{v}{Q^0} \pm \frac{M}{3} Q^1 \ln v\right).$$

Now that we have found the explicit form of S, we can use (5.3) to calculate

$$p_v = \frac{\partial S'}{\partial v} = -\frac{2M^2}{9}\frac{1}{Q^0} \pm \frac{M}{3}\frac{p_\phi}{v}, \tag{5.21}$$

$$P_0 = -\frac{\partial S'}{\partial Q^0} = -\frac{2M^2}{9}\frac{v}{(Q^0)^2}. \tag{5.22}$$

From equation (5.22) we can get

$$v = -\frac{9}{2M^2}P_0(Q^0)^2.$$

We can substitute (5.21) and (5.22) into (5.12) to get

$$H_\tau = P_0 \pm \frac{2}{3}\frac{Mp_\phi}{Q^0}. \tag{5.23}$$

This tells us that the physical Hamiltonian is

$$H = \pm\frac{2}{3}\frac{Mp_\phi}{Q^0}.$$

We can note here that the degrees of freedom of the system have been reduced by two [12]. First, we got rid of the variable N when we transformed to the variable τ. Then, v and p_v have been absorbed in the definition of Q^0.

Now, we can replace Q^0 with τ in the Hamiltonian and we can calculate the equations of motion:

$$\frac{dv}{d\tau} = \{v, H\} = 0,$$

$$\frac{d\phi}{d\tau} = \{\phi, H\} = \pm\frac{2M}{3\tau}.$$

From the equation of motion for ϕ we get

$$\phi(\tau) = \phi_0 \pm \frac{2M}{3}\ln\tau.$$

Now we can quantize trivially. Using the Hamiltonian (5.23) and choosing the representation $P_0 \to -i\hbar\frac{\partial}{\partial\tau}$, our wave function $\Psi(p_\phi, \tau)$ will obey a Schrödinger equation:

$$i\hbar\frac{\partial\Psi}{\partial\tau} = \pm\frac{2M}{3}\frac{p_\phi}{\tau}\Psi. \tag{5.24}$$

Solutions to this equation are of the form:

$$\Psi(p_\phi, \tau) = \Psi(p_\phi)\exp\left\{\mp\frac{2iM}{3\hbar}p_\phi\ln\tau\right\}$$

In this case, $\Psi(p_\phi)$ is a function that takes care of the normalization. So, here it would seem that we have obtained a legitimate time evolution for the wave function, which was our initial goal.

To verify it, let's try to calculate the average of the scalar field ϕ and compare the result to the one obtained classically:

$$\langle\phi\rangle = \langle\Psi|\,\phi\,|\Psi\rangle = i\int dp_\phi \Psi^*(p_\phi, \tau)\frac{\partial\Psi}{\partial p_\phi}(p_\phi, \tau)$$

So we get

$$\langle\phi\rangle = \pm\frac{2M}{3}\ln(\tau).$$

Deriving this with respect to time:

$$\langle\dot{\phi}\rangle = \pm\frac{2M}{3}\frac{1}{\tau} \tag{5.25}$$

On the other hand, the derivation of the classical equations of motion gave us our constraint, equation (5.6):

$$a^3\dot{\phi}^2 - M^2 a\dot{a}^2 = 0.$$

If we use the classical solution of the Friedmann equation $a(t) = a_0 t^{1/3}$, we get that the classical evolution of the scalar field is

$$\dot{\phi} = \pm\frac{M}{3t}.$$

So we can see that this doesn't coincide with (5.25). What have gone wrong here? We'll discuss it in the next sections.

5.3 Finding the time function by applying the constraint

The idea this time is to try again to find a time function but now instead of requiring that our function have Poisson bracket with the Hamiltonian equal to one in the whole phase space, we'll require it only in the constrained surface. We'll follow a slightly different procedure than in the last section, which we will discuss in detail in section 6.2. We'll also use Lagrangian (4.7) instead of (4.2), but the main ideas are the same.

We begin by taking again the metric of a flat FLRW universe coupled to a scalar field. This time we will parametrize the scale factor as $a(t) = e^{\alpha(t)}$. The corresponding Lagrangian is (4.7):

$$\mathcal{L} = -\frac{M^2\dot{\alpha}^2 e^{3\alpha}}{2N} + \frac{\dot{\phi}^2 e^{3\alpha}}{2N}.$$

In chapter 4 we calculated the conjugate momenta and the Hamiltonian corresponding to this Lagrangian. It reads:

$$H_D = N\left(-\frac{p_\alpha^2 e^{-3\alpha}}{2M^2} + \frac{p_\phi^2}{2}e^{-3\alpha}\right) = N\mathcal{H}.$$

The Hamiltonian constraint $\mathcal{H}$ vanishes weakly if we apply our constraint $p_N = 0$ (Note that $p_N = 0$ tells us that $p_\alpha^2/M^2 = p_\phi^2$). Of course, the vanishing of $\mathcal{H}$ means that also H_D vanishes weakly, as we would expect.

Now, as we did in the last section, we would like to find a dynamical time parameter: a function of the phase space variables. However, this time we won't derive our time function by solving the equations of motion, but instead we'll choose it by trying to do an educated guess.

For convenience, we'll choose our function in such a way that the time coincides with the cosmic time [22]. If we look at our flat FLRW metric, this is equivalent to setting the lapse function N to be equal to one. At the same time, this is equivalent to doing a gauge fixing of the type [30]

$$\chi(t, \alpha, p_\alpha, \phi, p_\phi) = t - \tilde{\chi}(\alpha, p_\alpha, \phi, p_\phi) = 0.$$

If we take the time derivative of the last equation we get

$$1 = N\{\tilde{\chi}, \mathcal{H}\}.$$

So, if we want to have $N = 1$, we have to choose $\tilde{\chi}$ in such a way that $\{\tilde{\chi}, \mathcal{H}\} = 1$.This coincides with the method discussed in the last sections.

As we mentioned before, this time we won't solve the equations of motion to find our time function. Instead, we are going to try choosing a function that depends only on α and p_α. We are going to try the following function [22]:

$$\tilde{\chi}(\alpha, p_\alpha) = -\frac{M^2 e^{3\alpha}}{3p_\alpha}.$$

Note that this function is different from the one that we found in the last section. Let's calculate its Poisson bracket with the super Hamiltonian constraint. It is not hard to find that

$$\{\tilde{\chi}, \mathcal{H}\} = \frac{1}{2}\left(1 + \frac{M^2 p_\phi^2}{p_\alpha^2}\right).$$

As we can see, the Poisson bracket are not equal to one. However, if we apply our constraint ($p_\alpha^2/M^2 = p_\phi^2$), we'll get that the Poisson bracket are equal to one.

We can ask whether applying the constraint at this point leads us to find a consistent time function or not. To check, let's take a look at the classical solution of the Friedmann equation that we found in chapter 4. It is:

$$a(t) = a_0 t^{1/3}.$$

This means that

$$\alpha(t) = \ln a_0 + \frac{1}{3}\ln t,$$

And $\dot{\alpha} = 1/3t$. Substituting the expressions for $\alpha(t)$ and $\dot{\alpha}$ into the expression for p_α and setting $N = 1$ we get

$$p_\alpha = -\frac{M^2 a_0^3}{3}.$$

Now, substituting $\alpha(t)$, $\dot{\alpha}$ and our last expression for p_α into $\tilde{\chi}(\alpha, p_\alpha)$, we get

$$\tilde{\chi}(\alpha, p_\alpha) = \frac{-\cancel{M^2 a_0^3} t}{-\cancel{3}\frac{\cancel{M^2 a_0^3}}{\cancel{3}}} = t.$$

Our function coincides with the cosmic time! This seems to gives us some reassurance that we are taking a correct path, since we recovered the classical time in this case.

Going back to our problem, now we want to write our Hamiltonian in the form (5.2). To do it, we are going to find our generating function $S(q, Q)$. Following equation (5.4) and writing $\tilde{\chi}(\alpha, p_\alpha)$ as a new variable that we'll call T, we find

$$T = \tilde{\chi}\left(\alpha, \frac{\partial S}{\partial \alpha}\right).$$

This means that we have to solve the following differential equation

$$\frac{dS}{d\alpha} = -\frac{M^2 e^{3\alpha}}{3T}.$$

The solution of this equation is

$$S(\alpha, T) = -\frac{M^2 e^{3\alpha}}{9T} + C.$$

Here, C is a constant of integration. Having found the generating function, we can calculate the conjugate momenta to the variable T:

$$P_T = -\frac{\partial S}{\partial T} = -\frac{p_\alpha^2 e^{-3\alpha}}{M^2}$$

Now we can make the transformation for the variables (α, p_α) to (T, P_T) in the Hamiltonian. To do it, begin by taking the original Hamiltonian

$$H_D = p_\alpha \dot{\alpha} + p_\phi \dot{\phi} - \mathcal{L}.$$

After doing the appropriate substitutions, simplifying and renaming the variable T as t to make the notation less cumbersome, we get

$$H_D = -\frac{Mp_\phi}{3t} - P_T.$$

We can now define the physical or reduced Hamiltonian:

$$H_{phys} = \frac{Mp_\phi}{3t}. \tag{5.26}$$

So that the total Hamiltonian reads

$$H_D = -P_T - H_{phys}.$$

Since H_D is constraint to vanish, we know that

$$P_T = -H_{phys}.$$

At this point we can now apply canonical quantization. By choosing the representaion $P_T \to -i\hbar\frac{\partial}{\partial t}$ we would get the following schrödinger equation for our wave function $\Psi(p_\phi, t)$:

$$i\hbar\frac{\partial\Psi}{\partial t} = \frac{Mp_\phi}{3t}\Psi.$$

Compare this with equation (5.24). The similarity is clear. This seems to tell us that we don't necessarily need to exclude the use of the constraint when looking for a dynamical time function in order to obtain a consistent Schrödinger equation.

5.4 Finding the time function without solving the equations of motions or applying the constraint

In the example we studied in section 5.2, we found a time function by solving the equations of motion and we made sure that this function had Poisson bracket with the Hamiltonian equal to one in the whole phase space. On the other hand, in section 5.3, we found a time function without solving the equations of motion and its Poisson bracket with the Hamiltonian was equal to one only in the constraint surface. However, we obtained similar results in both cases.

This time we are going to find a dynamical time function without solving the equations of motion, but making sure that its Poisson bracket with the Hamiltonian is equal to one in the whole phase space. Then, we will point out some apparent inconsistencies with what we have done in section 5.2.

We will maintain the notation of the last section. So that the Hamiltonian and the conjugate momenta are equal to those calculated before.

To begin, note that we can find a time function basically looking for a function of the phase space variables that has Poisson bracket with the Hamiltonian equal to 1 everywhere [12]. A function like this needs to depend on α, p_α and p_ϕ.

So, in principle there are not many more restrictions on the form that our time function should have. If we find some function of the phase space variables that has Poisson bracket with the Hamiltonian equal to one it should serve as a good time function. However, nothing really tells us that such a function is unique and, in fact, it's not [6].

To see this, let's try to choose the following function of the space time variables as our time function

$$T_p = \frac{2M^2 e^{3\alpha}}{3(Mp_\phi - p_\alpha)}. \tag{5.27}$$

Compare this with equation (5.17). Making the right substitutions we'll realize that they're similar with the exception of some constants and some signs.

It's not hard to verify that this function has Poisson bracket with the Hamiltonian equal to one in the whole phase space:

$$\{T_p, H\} = \frac{(Mp_\phi - p_\alpha)^2}{(Mp_\phi - p_\alpha)^2} = 1.$$

Note also that if we apply the constraint to T_p and choose $Mp_\phi = -p_\alpha$, it will reduce to the time function T introduced in the last section.

In fact, there is still another function that has Poisson bracket with the Hamiltonian equal to one and coincides with our time function T if we apply the constraint and choose $Mp_\phi = p_\alpha$. This function is:

$$T_{p1} = -\frac{2M^2 e^{3\alpha}}{3(Mp_\phi + p_\alpha)}.$$

This is an example of what we mentioned before. The time function is not unique, which is in agreement with the technical problem that we expect to appear in this kind of approach, the multiple choice problem [6].

In order to continue, we want to perform canonical quantization using T_p as our time function. We proceed as before. First, let us look for the conjugate momentum of the variable T_p. Let's find the generating function $S(q, Q)$:

$$T_p = f\left(\alpha, \frac{\partial S}{\partial \alpha}, \frac{\partial S}{\partial \phi}\right).$$

Which means that we have to solve the following differential equation:

$$M\frac{\partial S}{\partial \phi} - \frac{\partial S}{\partial \alpha} = \frac{2M^2 e^{3\alpha}}{3T_p}. \tag{5.28}$$

Here $S = S(\alpha, \phi, T_p, T_{p'})$ and T_p and $T_{p'}$ are constants of integration. So far this looks very much like what we did in section 5.2. However, as we saw, we must have overlooked some detail, since the average value of the field ϕ doesn't coincide with its classical value. To see what was exactly what we missed, let's solve the last differential equation carefully.

Let's begin by performing a change of variables:

$$u = \alpha + \frac{\phi}{M}, \qquad v = \alpha - \frac{\phi}{M}.$$

Then we will have

$$\phi = \frac{(u-v)M}{2}, \qquad \alpha = \frac{u+v}{2}.$$

Using the chain rule we get

$$M\frac{\partial S}{\partial \phi} = \frac{\partial S}{\partial u} - \frac{\partial S}{\partial v}, \qquad \frac{\partial S}{\partial \alpha} = \frac{\partial S}{\partial u} + \frac{\partial S}{\partial v}.$$

Then, we can write the differential equation (5.28) in the new variables as

$$\frac{\partial S}{\partial v} = -\frac{M^2 \exp\left\{\frac{3}{2}(u+v)\right\}}{3T_p}.$$

This can be integrated immediately to give

$$S = -\frac{2M^2 \exp\left\{\frac{3}{2}(u+v)\right\}}{9T_p} + \tilde{f}(u).$$

Here, $\tilde{f}(u)$ is an arbitrary function of u. Going back to our original variables, the result looks like

$$S = -\frac{2M^2 e^{3\alpha}}{9T_p} + \tilde{f}\left(\alpha + \frac{\phi}{M}\right).$$

Now that we have the generating function, we can find the conjugate momentum of T_p by deriving S with respect to T_p. However, we have to be careful here. Our arbitrary function depends on α. And at the same time, T_p is related to α via equation (5.27). In fact, using (5.27) we can write S as

$$S = -\frac{2M^2 e^{3\alpha}}{9T_p} + \tilde{f}\left(\frac{\phi}{M} + \frac{1}{3}\ln\left\{\frac{3T_p(Mp_\phi - p_\alpha)}{2M^2}\right\}\right). \tag{5.29}$$

To make the notation less cumbersome, we are going to define

$$z(T_p) = \frac{1}{3}\ln\left\{\frac{3T_p(Mp_\phi - p_\alpha)}{2M^2}\right\} \tag{5.30}$$

So that we can write equation (5.29) like

$$S = -\frac{2M^2e^{3\alpha}}{9T_p} + \tilde{f}\left(\frac{\phi}{M} + z(T_p)\right). \tag{5.31}$$

Now we can finally calculate the conjugate momentum P_{T_p}. To do it we take the derivative of S with respect to T_p:

$$P_{T_p} = -\frac{\partial S}{\partial T_p} = -\frac{2M^2e^{3\alpha}}{9T_p^2} - \frac{\partial\tilde{f}}{\partial z}\frac{\partial z}{\partial T_p}.$$

Taking the derivative of (5.30) with respect to T_p we get

$$P_{T_p} = -\frac{2M^2e^{3\alpha}}{9T_p^2} - \frac{1}{3T_p}\frac{\partial\tilde{f}}{\partial z}.$$

Substituting equation (5.27) and rearranging a bit we get

$$P_{T_p} = \frac{e^{-3\alpha}}{M^2}\left[-\frac{1}{2}(Mp_\phi - p_\alpha)^2 - \frac{1}{2}(Mp_\phi - p_\alpha)\frac{\partial\tilde{f}}{\partial z}\right]. \tag{5.32}$$

This tells us that P_{T_p} is not uniquely defined. Its final form will depend on how exactly our function $\tilde{f}$ depends on z, which we didn't notice in the calculations we performed in the preceding sections.

To advance further, we are going to pick a specific form for the term $\frac{\partial\tilde{f}}{\partial z}$, seeking however to keep some of the freedom that the arbitrariness of $\tilde{f}$ gives us. Because it will allow us to obtain simple expressions that we can compare with what we have already obtained in the pasts sections, let us choose

$$\frac{\partial\tilde{f}}{\partial z} = -\left(2\frac{A}{M} + M\right)p_\phi.$$

In this case, A is an arbitrary constant. Substituting this in equation (5.32) we get that the conjugate momentum of T_p is

$$P_{T_p} = \frac{e^{-3\alpha}}{M^2}\left(-\frac{1}{2}p_\alpha^2 + Ap_\phi^2 + \left(\frac{M}{2} - \frac{A}{M}\right)p_\phi p_\alpha\right). \tag{5.33}$$

Now that we have P_{T_p}, we want to get the reduced Hamiltonian, that we will call H_{phy-p}. To do it, subtract (5.33) from the Hamiltonian, remembering that we have chosen $N = 1$. We get

$$H_{phy-p} = \frac{(M^2 - 2A)(Mp_\phi - p_\alpha)e^{-3\alpha}p_\phi}{2M^3}.$$

We can use the definition of T_p to get rid of the factor of $e^{-3\alpha}$ in the reduced Hamiltonian:

$$H_{phy-p} = \frac{(M^2 - 2A)p_\phi}{3MT_p}.$$

Now we just have to make the substitution $T_p = t$:

$$H_{phy-p} = \frac{(M^2 - 2A)p_\phi}{3Mt}. \tag{5.34}$$

Compare this expression with the physical Hamiltonian obtained in the last section. The two expressions have the same form. In fact, for $A = 0$ we recover H_{phys}. It is interesting that we can get a similar Hamiltonian in both cases, since in the present case we obtained this expression without using the constraint and requiring that the Poisson bracket are equal to one in all the phase space and not only in the constraint surface.

But the most important feature of expression (5.34) is that it has a free parameter A. Note that we would obtain the results that we derived in section 5.2 if we put $A = -\frac{M^2}{2}$.

Expression (5.34) seems to tell us that, for the same choice of the classical cosmic time, there is whole family of different Hamiltonians: one for each possible value of A. Each of this Hamiltonians would give rise to a different time evolution of our system, meaning that we have a different physics for each choice of A, which is not physical.

However, there might be a way out of this problem. If we are able to somehow fix A, we would have a unique Hamiltonian. To investigate if can fix the value of A, let us begin by writing the corresponding Schrödinger equation:

$$i\hbar\frac{\partial\Psi}{\partial t}(p_\phi, t) = \frac{(M^2 - 2A)}{3Mt}p_\phi\Psi(p_\psi, t)$$

The solution of this equation is

$$\Psi(p_\psi, t) = \Psi(p_\phi)\exp\left\{-i\frac{(M^2 - 2A)p_\phi}{3M}\ln t\right\}.$$

Here, $\Psi(p_\phi)$ takes care of the normalization. We can calculate, for example, the average value of the momentum

$$\langle p_\phi\rangle = \langle\Psi|\,\phi\,|\Psi\rangle = \int dp_\phi p_\phi \Psi^*(p_\phi)\Psi(p_\phi).$$

This average value doesn't depend on time, just like its classical analogue. We can also calculate the average value of the scalar field ϕ:

$$\langle \phi \rangle = \langle \Psi | \, \phi \, | \Psi \rangle = i \int dp_\phi \Psi^*(p_\phi, t) \frac{\partial \Psi}{\partial p_\phi}(p_\phi, t).$$

So we get

$$\langle \phi \rangle = \frac{(M^2 - 2A)}{3M} \ln(t).$$

Deriving this with respect to time:

$$\langle \dot{\phi} \rangle = \frac{(M^2 - 2A)}{3Mt}. \tag{5.35}$$

We can compare equation (5.35) with the classical evolution of the scalar field ϕ. Remember that the constraint tells us that $M^2 \dot{\alpha}^2 = \dot{\phi}^2$. We'll choose the positive solution and we'll also remember that for $a(t) = a_0 t^{1/3}$ we have $\dot{\alpha} = \frac{1}{3t}$. Substituting this in the constraint we get that

$$\dot{\phi} = \frac{M}{3t}.$$

This is compatible with (5.35) only if

$$A = 0. \tag{5.36}$$

This incompatibility is of course a problem, because if A is different from equation (5.36) we have that the average value of the time derivative of the scalar field doesn't obey the equations derived classically from the Lagrangian. However, there is one last hope: we derived the family of Hamiltonians without imposing the constraint and we are comparing our result to what the constraint tells us. So, we can think that $\langle \dot{\phi} \rangle$ might coincide with the classical evolution of the field derived without imposing the constraint.

Let's give it a try. To simplify the notation, we'll fix $N = 1$. We'll also use the variable $a(t)$ instead of $\alpha(t)$. So the Lagrangian will be (4.2):

$$\mathcal{L} = -\frac{M^2 \dot{a}^2 a}{2} + \frac{\dot{\phi}^2 a^3}{2}.$$

The Klein-Gordon equation, as we saw on chapter 4 is just $\dot{\phi} a^3 = p_\phi =$ constant. Performing variations in the action with respect to $a(t)$ we get

$$M^2 \frac{d}{dt}(\dot{a} a) = -M^2 \frac{\dot{a}^2}{2} + \frac{3}{2} a^2 \dot{\phi}^2.$$

To solve this equation we'll introduce a new variable $x = a^{2/3}$. Our equation now will look like

$$\ddot{x} + \frac{9}{4}\frac{p_\phi^2}{M^2 x^3} = 0.$$

Integrating one time we get

$$\dot{x}^2 - \frac{3}{8}\frac{p_\phi^2}{M^2}\frac{1}{x^2} = C.$$

Here, C is an arbitrary constant. If $C = 0$ our constraint is satisfied. If $C \neq 0$ we can integrate again and get

$$x^2 = a^3 = \frac{3p_\phi t}{M} + Ct^2.$$

Using the Klein Gordon equation we get

$$\dot{\phi} = \frac{p_\phi}{\frac{3p_\phi t}{M} + Ct^2}.$$

This is incompatible with (5.35) for $C \neq 0$. So, even if we don't impose the constraint the classical evolution we just derived classically doesn't coincide with the one derived from our quantization method.

So, if we choose a parameter $A \neq 0$, the evolution of the quantum scalar field won't coincide with its classical analogue, just like it happened in our example in section 5.2.

5.5 Discussion

Equation (5.35) has a free parameter A, which means we have a family of Hamiltonians, each of them describing a different physics. In this case, when we try to change variables from (α, p_α) to (T_p, P_{T_p}), the conjugate momentum to the time variable is not unique, causing the Hamiltonian to have a dependence in the parameter A.

There is no easy criteria that allow us to pick one A over other one. The closest that we have to a criteria is to ask that the mean value of $\dot{\phi}$ coincides with that derive classically. This criteria can be justified by noting that the problem of the family of Hamiltonians seems to arise from the fact that we chose a time function that is valid in the whole phase space [12]. Since not all the points of the phase space represent physical solutions of our system, but only those that are on the constrained surface [8], we might think that also not all the Hamiltonians in this family are going to give us a physical evolution, and that we should choose the one that corresponds to the constraint surface.

In general, and as anticipated in chapter 3, we saw that the time function is not unique. There is more than one phase space function that can serve as time and that have Poisson bracket with the Hamiltonian equal to 1. This is the multiple choice problem [6], one of the main problems that this kind of approach to the problem of time presents.

Chapter 6

Born-Oppenheimer approach and gauge fixing

In chapter 3 we mentioned briefly the semiclassical interpretation of quantum gravity as one of the approaches to the problem of time in the Wheeler-DeWitt framework [4]. One of the approaches that is usually used in combination with the semiclassical interpretation is the Born-Oppenheimer (BO) approach [42]. The BO approach introduces the idea that time emerges only when a state of our quantum system becomes classical. This means that not all solutions to the Wheeler-DeWitt equation allow a dynamical interpretation [6].

On the other hand, in chapter 5 we saw that we can introduce time in our formalism by doing a gauge fixing of the type

$$\chi(t, \alpha, p_\alpha, \phi, p_\phi) = t - \bar{\chi}(\alpha, p_\alpha, \phi, p_\phi) = 0.$$

If one applies the BO approach and the gauge fixing method to the model we studied in the last chapter (flat FLRW spacetime coupled to a scalar field), we find that the results are similar for both approaches [22]. This can led us to consider whether there is some kind of connection between the BO approach and the gauge fixing method. A possible answer to this question was given in a recent paper by Chataignier [43], where it is argued that the results of the semiclassical approach can be obtained from a particular gauge fixing.

In the present chapter, we review the basics of the BO approach and apply it to the model under study. We then discuss the gauge fixing approach [30] and compare the results obtained by this method with those obtained using the BO approach. Finally, taking as a starting point the paper by Chataignier [43], we explore the possible connection between the BO approach and the Gauge fixing method. We will explicitly write the Planck mass in our equations, since it will play a fundamental role in our arguments and approximations.

6.1 The Born-Oppenheimer approach to the problem of time

The Born-Oppenheimer approach was born as a method to treat composite molecule systems [44]. Composite systems are those that involve two very different mass or time scales. In particular, in a molecule system we have electrons and the nuclei, which have very different masses, making this system suitable for a BO approach.

The two different scales of the masses of the nuclei and electrons allows us to factorise the wave function on the system in a way that lead us, at first order, to a separate description of the behaviour of the nucleus and the electrons surrounding it. It also found that the motion of the nuclei is influenced by the mean Hamiltonian of the electrons [44].

In the case of a quantum minisuperspace coupled with matter we also have two very different scales, since the gravitational degrees of freedom are characterized by the Planck mass, which is much bigger than the usual matter mass scale [45]. In this sense, the gravitational degrees of freedom are "heavy", while the matter degrees of freedom are "light".

This approach is useful to analyse the emergence of time in the context of a semiclassical approximation for quantum gravity starting from a minisuperspace model describing gravity and quantum matter [11, 45, 46].

The BO approach tells us that not all the solutions to the Wheeler-DeWitt equation allow a dynamical interpretation, but that time and quantum dynamics emerge only when a state of our system becomes semiclassical [6].

If we focus on a composite system of a "heavy" sector interacting with a "light" subsystem, where the heavy sector is associated with a mass scale M and degrees of freedom Q_a, with $a = 1, ..., n$, and the light system is associated with a scale $m << M$ and degrees of freedom q_μ with $\mu = 1, ..., d$, we can expand the wave function as the superposition [43, 45]:

$$\Psi(Q; q) = \sum_k \varphi_k(Q)\chi_k(Q; q). \tag{6.1}$$

Here, the χ_k form a complete system, which is orthonormal with respect to the inner product taken only over the matter variables [45].

For simplicity, we can also rewrite equation (6.1) as [43]

$$\Psi(Q; q) = \varphi(Q) \sum_k \frac{\varphi_k(Q)}{\varphi(Q)}\chi_k(Q; q) = \varphi(Q)\chi(Q; q). \tag{6.2}$$

This exact factorization has the advantage that we don't have to consider the dynamics of each of the χ_k states. After factorizing the wavefunction in this way, the usual procedure of the BO approach is to insert this factorization in the Wheeler-DeWitt equation, multiply the result by χ^* and integrate over the light variables to obtain an equation for ϕ [22]. This equation will involve the partial average of the matter Hamiltonian.

The next step is to use the equation for ϕ to obtain an equation for χ, which will also involve partial averages with respect to the light sector. At this point, we can use the gravitational degrees of freedom to define a time parameter and obtain a Schrödinger equation for the light system. This means that the gravitational degrees of freedom provide the clock that parametrises the evolution of the light sector [22]. Let's see how this works in the case of a flat FLRW quantum cosmology.

6.1.1 BO approach for a flat FLRW quantum cosmology

We have already seen that in the case we have studied in the last two chapters the Wheeler-DeWitt equation is

$$\left(\frac{\partial^2}{\partial\alpha^2} + M^2\, p_\phi^2\right)\Psi(\alpha, p_\phi) = 0.$$

We now want to apply the BO approach to quantum gravity to this model. Following our past discussion, we are going to consider that the solution to this equation can be written in the following form [22, 43]

$$\Psi(\alpha, p_\phi) = \varphi(\alpha)\chi(\alpha, p_\phi). \tag{6.3}$$

At this point, it is useful to remember that the main idea of the BO approach is that time emerges when a state of our system is classical [4, 6, 45]. In this case, we are going to keep the gravitational degrees of freedom classical and the matter degrees of freedom will be quantized.

If we substitute equation (6.3) in the Wheeler-DeWitt equation we get:

$$\frac{\partial^2\varphi}{\partial\alpha^2} + 2\frac{\partial\varphi}{\partial\alpha} + \varphi\frac{\partial^2\chi}{\partial\alpha^2} + M^2 p_\phi^2\varphi\chi = 0. \tag{6.4}$$

To proceed further, we have to suppose two things. The first one is that the term $\varphi\frac{\partial\chi^2}{\partial\alpha^2}$ is small, so we can omit it [22]. The second one is that the partial average

$$\langle\chi|\frac{\partial\chi}{\partial\alpha}\rangle = 0. \tag{6.5}$$

Now, multiply equation (6.4) by χ^* to get

$$\frac{\partial^2\varphi}{\partial\alpha^2} + 2\chi^*\frac{\partial\varphi}{\partial\alpha}\frac{\partial\chi}{\partial\alpha} + M^2 p_\phi^2\varphi = 0.$$

We can take now the average of this equation with respect to the matter sector in order to get an equation for $\varphi(\alpha)$:

$$\frac{\partial^2 \varphi}{\partial \alpha^2} + M^2 \langle p_\phi^2 \rangle \varphi = 0.$$

This equation can be easily integrated to get

$$\varphi(\alpha) = \exp\Big(-iM\sqrt{\langle p_\phi^2 \rangle}\alpha\Big). \tag{6.6}$$

Substitute equation (6.6) into equation (6.4). Neglecting $\varphi \frac{\partial^2 \chi}{\partial \alpha^2}$ we get

$$-M^2 \langle p_\phi^2 \rangle \chi - 2iM\sqrt{\langle p_\phi^2 \rangle} \frac{\partial \chi}{\partial \alpha} + M^2 p_\phi^2 \chi = 0. \tag{6.7}$$

In chapter 4, we found that $p_\phi = e^{3\alpha}\dot{\phi}$ and we saw that the constraint is $M^2 \dot{\alpha}^2 = \dot{\phi}^2$. So, we can write $\dot{\alpha}$ in terms of p_ϕ:

$$\dot{\alpha} = \frac{p_\phi e^{-3\alpha}}{M}. \tag{6.8}$$

We are now going to introduce a semiclassical cosmic time parameter. To do it, substitute the classical right hand side of equation (6.8) by the partial average of the corresponding operator [22] to get

$$\dot{\alpha} = \frac{\sqrt{\langle p_\phi^2 \rangle} e^{-3\alpha}}{M}. \tag{6.9}$$

Using equation (6.9) to rewrite equation (6.7) we get

$$-\langle p_\phi^2 \rangle \chi - 2ie^{3\alpha}\dot{\alpha}\frac{\partial \chi}{\partial \alpha} + p_\phi^2 \chi = 0. \tag{6.10}$$

Note that

$$\dot{\alpha}\frac{\partial \chi}{\partial \alpha} = \frac{\partial \chi}{\partial t}.$$

Using this, we can rewrite equation (6.10) as

$$-\langle p_\phi^2 \rangle \chi - 2ie^{3\alpha}\frac{\partial \chi}{\partial t} + p_\phi^2 \chi = 0. \tag{6.11}$$

Equation (6.11) can be rearranged to give

$$i\frac{\partial \chi}{\partial t} = \frac{p_\phi^2}{2} e^{-3\alpha}\chi - \frac{\langle p_\phi^2 \rangle}{2} e^{-3\alpha}\chi.$$

All we have to do now is to remember that $\frac{p_\phi^2}{2}e^{-3\alpha}$ is the term in the Hamiltonian corresponding to the matter degrees of freedom. We can call it H_m, so that we can write the last equation as

$$i\frac{\partial\chi}{\partial t} = H_m\chi - \langle H_m\rangle\chi. \tag{6.12}$$

Equation (6.12) is a Schrödinger-like equation. We can recover Schrödinger's equation by making the phase transformation [22]:

$$\chi = \tilde{\chi}\exp\left(i\int\langle H_m\rangle dt\right).$$

Substituting this expression into equation (6.12) we get the time-dependent Schrödinger equation:

$$i\frac{\partial\tilde{\chi}}{\partial t} = H_m\tilde{\chi}. \tag{6.13}$$

6.2 Gauge fixing approach to the problem of time

The Gauge fixing approach to the problem of time was described in detail in [30]. In this section, we will review its main ideas, which we have partially discussed in chapter 5.

We mentioned at the beginning of this chapter that not all solutions to the Wheeler-DeWitt equation allow a dynamical interpretation. In fact, the Wheeler-DeWitt equation has solutions that don't correspond to the physical set up we are attempting to describe [4, 6, 7]. Having this in mind,we need some additional criterium in order for us to extract the physical solutions and distinguish them from the non-physical ones.

In [30] it is proposed that a way to extract the physical solutions can consist in the so-called reduced space quantization or gauge fixing. The main idea of this phase space reduction is the selection of time parameter as a function of the phase space variables. Choosing a time parameter allows us to find the physical degrees of freedom and their Hamiltonian while at the same time introducing evolution of the quantum states. Let's see how this works in the general case.

In general, the action of a gravity theory has the form [30]

$$S = \int dt(p_i\dot{q}^i - N^\mu H_\mu(q,p))$$

As before, N_μ are the lapse and shift functions. Variations with respect to N_μ leads to our well-known Hamiltonian and diffeomorphism constraints

$$H_\mu(q,p) = 0.$$

A theory of this type is invariant under diffeomorphisms [7]. This means that we can have a set of states that at first seem to be different from each other but in reality they are related by transformations of coordinates and they all represent the same physical state [30]. The idea of the physical reduction is to choose one representative of this physical state and treat the labels of this state as physical variables.

We can do this by imposing on the phase space variables the following gauge conditions [30]

$$\chi^{\mu}(q,p,t)=0. \tag{6.14}$$

For systems that are invariant under diffeomorphisms the gauge condition should explicitly depend on time in order to generate the dynamics in the phase space [30]. Using these gauge conditions we can fix the shift and the lapse functions by requiring the conservation of equation (6.14) in time:

$$\frac{d\chi^{\mu}}{dt}=\frac{\partial\chi^{\mu}}{\partial t}+\{\chi^{\mu},H_{\nu}\}N^{\nu}=0. \tag{6.15}$$

We can define the matrix

$$J^{\mu}{}_{\nu}=\{\chi^{\mu},H_{\nu}\}.$$

So that we can write the lapse and the shift functions as

$$N^{\mu}=-(J^{\mu}{}_{\nu})^{-1}\frac{\partial\chi^{\nu}}{\partial t}. \tag{6.16}$$

The next step is to write the phase space variables (q^i,p_i) in terms of the new variables of the physical sector, that we'll call (ξ^A,π_A). Solving the systems of constraints and the gauge conditions we can write

$$\begin{aligned} q^i &= q^i(\xi^A,\pi_A,t),\\ p_i &= p_i(\xi^A,\pi_A,t). \end{aligned}$$

This change of coordinates is given by a canonical transformation that should obey [30]

$$p_i dq^i=\pi_A d\xi^A-H_{phys}(\xi^A,\pi_A,t)dt+dF(q^i,\xi^A,t). \tag{6.17}$$

Here, $H_{phys}(\xi^A,\pi_A,t)$ is considered to be the physical Hamiltonian and $F(q^i,\xi^A,t)$ is the generating function of this canonical transformation.

Once we have found the physical Hamiltonian we can perform canonical quantization by promoting the variables ξ^A and π_A and the physical Hamiltonian to operators:

$$\xi^A,\longrightarrow\hat{\xi}^A,\qquad \pi_A\longrightarrow\hat{\pi}_A\qquad H_{phys}\longrightarrow\hat{H}_{phys}.$$

The physical variables are subjected to the usual commutation relation

$$[\hat{\xi}^A, \hat{\pi}_B] = i\hbar\delta^A_B.$$

Finally, we postulate the Schödringer equation for the physical states

$$i\hbar\frac{\partial}{\partial t}\Psi_{phys}(t,\xi) = \hat{H}_{phys}\Psi(t,\xi). \tag{6.18}$$

In the particular case of minisuperspace models,the diffeomorphism constraints are satisfied automatically and we remain only with the Hamiltonian constraint. So that we'll have [4, 6, 30]

$$H_\mu(q,p) = H(q,p), \qquad\qquad \chi^\mu(q,p,t) = \chi(q,p,t).$$

In this case, we can write the gauge condition to express time explicitly as a function of the phase space variables [30]

$$\chi(q,p,t) = T(q,p) - t = 0. \tag{6.19}$$

We can then fix the lapse function

$$N = \frac{1}{J}.$$

Here, $J = \{T, H\}$. In minisuperspace models, the gravitational degrees or freedom are given by the scale factor $a = e^\alpha$ so that our phase space variables are

$$q^i, p_i = \alpha; p_\alpha, \xi, \pi.$$

In this equation, ξ and π are matter degrees of freedom. After fixing a gauge of the form given by equation (6.19), we need to find a a canonical transformation $F(\alpha, T)$ that takes us from the variables (α, p_α) to (T, p_T), where $T = T(\alpha, p_\alpha)$ and $p_T = p_T(\alpha, p_\alpha)$. Once we have changed variables, the Hamiltonian constraint and the Wheeler-DeWitt equation read [30]

$$H(T, p_T; \xi, \pi) = 0,$$
$$\hat{H}\left(T, i\frac{\partial}{\partial T}; \hat{\xi}, \hat{\pi}\right)|\Psi_{phys}(T)\rangle = 0.$$

The wavefunction $|\Psi_{phys}(t)\rangle$, obeys the Schrödinger equation. We have already seen this formalism in action in our case of study on section 5.3, where we picked a gauge that coincides with the classical solution of the Friedmann equation. In this case, we found that the resulting wavefunction obeys the Schrödinger equation, giving an example of how this formalism works.

6.3 The relationship between the BO approach and Gauge fixing

Taking inspiration from the paper by Chataignier [43], we now set to find a connection between the Born-Oppenheimer approach to quantum gravity and gauge fixing. The question if there is a connection between the Born-Oppenheimer approach and the gauge fixing method was posed in a recent paper by Kamenshchik, Tronconi, Vardanyan and Venturi [22], where similar results are obtained for both approaches.

In the gauge fixing method, we chose a time variable as a function of the phase space variables. This allowed us to fix the value of the lapse N. The time variable is usually chosen in such a way that the lapse is equal to 1, since this gives us that the cosmic time coincides with the usual time.

On the other hand, in the Born-Oppenheimer approach, we make the assumption that we can write the wave function as $\Psi(\alpha, p_\phi) = \varphi(\alpha)\chi(p_\phi, \alpha)$ where ϕ depends only on the gravitational degrees of freedom, and χ can depend on both the gravitational and matter degrees of freedom [45]. In this case, a function of α serves as an internal clock for the system, allowing for a definition of time.

In this case, we are going to pick a particular gauge and find the lapse function associated to it. This lapse function instead of being a constant is going to be a function of the phase space variables. After this, we are going to use the newly define variables to find the Schrödinger equation, which in this case will coincide with the one found in the case of a pure BO approach. We'll also see that if we start from the Wheeler-DeWitt equation we can also find the BO ansatz if we perform a phase transformation, using as a phase the generating function of the change of variables. Let's see how this works.

6.3.1 BO approach from gauge fixing: classical theory

We begin with the usual metric

$$ds^2 = N^2(t)dt^2 - a^2(t)(dx^2 + dy^2 + dz^2).$$

Coupled to a scalar field ϕ. In this case, following Chataignier [43], we will include the cosmological constant, in order to have a nonzero gravitational potential. The Lagrangian for this theory is:

$$\mathcal{L} = -M^2 \frac{a\dot{a}^2}{N} - M^2 \frac{\Lambda}{6} N a^3 + \frac{a^3 \dot{\phi}^2}{2N}.$$

Here, Λ is the cosmological constant and M is the re-scaled Planck mass. If we parametrize the scale factor as $a(t) = e^{\alpha(t)}$ the Lagrangian is

$$\mathcal{L} = -\frac{M^2 \dot{\alpha}^2 e^{3\alpha}}{2N} - \frac{\Lambda}{6} M^2 N e^{3\alpha} + \frac{e^{3\alpha}\dot{\phi}^2}{2N}.$$

The conjugate momenta are

$$p_N = 0, \qquad\qquad p_\alpha = -\frac{M^2\dot{\alpha}e^{3\alpha}}{N}, \qquad\qquad p_\phi = \frac{e^{3\alpha}\dot{\phi}}{N}.$$

Using the conjugate momenta, we can now write the Hamiltonian

$$H = p_\alpha\dot{\alpha} + p_\phi\dot{\phi} - \mathcal{L}.$$

The result is

$$H = N\left(-\frac{p_\alpha^2 e^{-3\alpha}}{2M^2} + \frac{p_\phi^2}{2}e^{-3\alpha} + \frac{\Lambda}{6}M^2 e^{3\alpha}\right). \tag{6.20}$$

The Hamiltonian constraint then is [43]

$$H = H_g(\alpha, p_\alpha) + H_m(\alpha, p_\phi) = 0.$$

Here, H_g is the gravitational Hamiltonian and H_m is the matter Hamiltonian. The cosmological constant can be treated either as an element of the gravitational Hamiltonian or as a part of the matter Hamiltonian. In the last case, it would be interpreted as the scalar field potential. Following [43], we decide to treat it as a part of the gravitational Hamiltonian. We then have

$$\begin{aligned} H_g &= -\frac{p_\alpha^2 e^{-3\alpha}}{2M^2} + \frac{\Lambda}{6}M^2 e^{3\alpha}, \\ H_m &= \frac{p_\phi^2}{2}e^{-3\alpha}. \end{aligned}$$

Simplifying, the constraint reads

$$-\frac{p_\alpha^2}{M^2} + p_\phi^2 + \frac{\Lambda}{3}M^2 e^{6\alpha} = 0. \tag{6.21}$$

Now, we will impose the following gauge condition [43]

$$\chi(\alpha, t) = \alpha - t = 0. \tag{6.22}$$

To fix the lapse function, we require that the gauge condition be conserved at all times [30]

$$\frac{d\chi}{dt} = \frac{\partial\chi}{\partial t} + N\{\chi, H\} = 0.$$

We can calculate the Poisson bracket of the gauge condition with the Hamiltonian to get

$$\{\chi, H\} = \frac{e^{-3\alpha}p_\alpha}{M^2}.$$

Substituting in the conservation equation, we get that the lapse function is

$$N = \frac{M^2 e^{3\alpha}}{p_\alpha}. \tag{6.23}$$

Solving the Hamiltonian constraint, we get

$$p_\alpha = \pm M\left(p_\phi^2 + \frac{\Lambda}{3}e^{6\alpha}M^2\right)^{1/2}. \tag{6.24}$$

We can substitute equation (6.24) in (6.23) to get

$$N = \pm\frac{Me^{3\alpha}}{\left(p_\phi^2 + \frac{\Lambda}{3}e^{6\alpha}M^2\right)^{1/2}}.$$

We can rearrange the denominator and expand it in powers of $\frac{1}{M^2}$ to obtain

$$N = \pm\sqrt{\frac{3}{\Lambda}}\left(1 - \frac{3p_\phi^2 e^{-6\alpha}}{2\Lambda M^2} + ...\right).$$

At first order the lapse is

$$N = \pm\sqrt{\frac{3}{\Lambda}} + O\left(\frac{1}{M^2}\right). \tag{6.25}$$

With the lapse fixed, we can go back to equation (6.24) and expand the negative square root in powers of $\frac{1}{M^2}$ to get, at first order

$$p_\alpha = -\sqrt{\frac{\Lambda}{3}}M^2 e^{3\alpha} - \sqrt{\frac{3}{\Lambda}}\frac{p_\phi^2}{2}e^{-3\alpha} + O\left(\frac{1}{M^2}\right). \tag{6.26}$$

Our gauge fixing induces a canonical transformation with generating function

$$\varphi(\alpha) = -\frac{1}{3}\sqrt{\frac{\Lambda}{3}}M^2 e^{3\alpha}. \tag{6.27}$$

So that the relationship between p_α and p_t is

$$p_t = p_\alpha - \frac{d\varphi}{dt}. \tag{6.28}$$

We can substitute equation (6.28) in equation (6.26) to get

$$p_t = -\sqrt{\frac{3}{\Lambda}}\frac{p_\phi^2}{2}e^{-3\alpha} + O\left(\frac{1}{M^2}\right) = NH_m. \tag{6.29}$$

We can proceed now to quantize equation (6.29). Using a mixed representation where

$$\hat{p}_t\Psi = -i\frac{\partial\Psi}{\partial t}, \qquad \hat{p}_\phi\Psi = p_\phi\Psi.$$

We get Schrödinger's equation:

$$i\frac{\partial\Psi}{\partial t} = \sqrt{\frac{3}{\Lambda}}\frac{p_\phi^2}{2}e^{-3\alpha}\Psi.$$

This is the result we got for the BO approach, multiplied by the value of the lapse function at first order.

6.3.2 Quantum theory

We can also get the result of the BO approach starting from the Wheeler-DeWitt equation instead of the classical theory [43], as we did in the last subsection. To do it, we begin with Hamiltonian (6.20) and promote the variables to operators. We choose to work in a mixed representation where

$$\hat{\alpha}\Psi(\alpha, p_\phi) = \alpha\Psi(\alpha, p_\phi), \qquad \hat{p}_\alpha\Psi = -i\frac{\partial\Psi}{\partial\alpha}, \qquad \hat{p}_\phi\Psi = p_\phi\Psi.$$

Here, $\Psi(\alpha, p_\phi)$ is the wavefunction of the universe. It is convenient to work in this representation, since p_ϕ is conserved. Using this representation, the Wheeler-DeWitt equation, $\hat{H}\Psi = 0$, reads

$$\frac{e^{-3\alpha}}{2M^2}\frac{\partial^2\Psi}{\partial\alpha^2} + \frac{e^{-3\alpha}}{2}p_\phi^2\Psi + \frac{\Lambda}{6}M^2e^{3\alpha}\Psi = 0. \tag{6.30}$$

To recover the Schrödinger equation, we perform the phase transformation [43] $\Psi(\alpha, p_\phi) = e^{i\varphi(\alpha)}\Psi_\varphi$ where $\varphi(\alpha)$ is the generating function of the transformation [43] we used in the classical treatment of the system, given by equation (6.27).

After performing the phase transformation and taking the appropriate derivatives, equation (6.30) reads

$$-i\sqrt{\frac{\Lambda}{3}}\frac{\partial\Psi_\varphi}{\partial\alpha} = -\frac{e^{-3\alpha}}{2}p_\phi^2\Psi_\varphi - \frac{\sqrt{3\Lambda}}{2}i\Psi_\varphi + \frac{e^{-3\alpha}}{2M^2}\frac{\partial^2\Psi_\varphi}{\partial\alpha^2} \tag{6.31}$$

To the lowest order this equation reads

$$i\frac{\partial\Psi_\varphi}{\partial\alpha}=\sqrt{\frac{3}{\Lambda}}\frac{p_\phi^2}{2}e^{-3\alpha}\Psi_\varphi-\frac{3}{2}i\Psi_\varphi+O\left(\frac{1}{M_{pl}^2}\right). \tag{6.32}$$

Equation (6.32) almost looks like the Schrödinger equation. However, we have an imaginary constant on the right hand side. This is a problem because it ruins unitarity. Is there any way we can enforce unitarity in this equation? To answer this question, write the wavefunction as

$$\tilde{\Psi}_\varphi=e^{-3/2\alpha}\Psi_\varphi. \tag{6.33}$$

Substituting equation (6.33) into equation (6.32) we get

$$i\frac{\partial\tilde{\Psi}_\varphi}{\partial\alpha}=\sqrt{\frac{3}{\Lambda}}\frac{p_\phi^2}{2}e^{-3\alpha}\tilde{\Psi}_\varphi+O\left(\frac{1}{M^2}\right). \tag{6.34}$$

This is the same result we got in the last section. Note that the transformation of the wavefunction performed in equation (6.33) can be written as

$$\tilde{\Psi}_\varphi(\alpha,p_\phi)=e^{i\varphi(\alpha)}e^{-3/2\alpha}\Psi_\varphi(\alpha,p_\phi)=\chi(\alpha)\Psi_\varphi(\alpha,p_\phi).$$

This is the BO approach ansatz [22, 43, 45]. So, in this sense, by fixing a gauge, we have recovered the main ansatz of the BO approach.

We also introduce the backreaction [45] (the average of the matter Hamiltonian) in these equations. By taking the average of equation (6.31) with respect to the matter sector we find

$$i\langle\frac{\partial}{\partial\alpha}\rangle\Psi_\varphi-\sqrt{\frac{3}{\Lambda}}\frac{\langle p_\phi^2\rangle}{2}e^{-3\alpha}\Psi_\varphi-\frac{3}{2}i\Psi_\varphi+\sqrt{\frac{3}{\Lambda}}\frac{e^{-3\alpha}}{2M^2}\langle\frac{\partial^2}{\partial\alpha^2}\rangle\Psi_\varphi=0. \tag{6.35}$$

We can define

$$\frac{\langle p_\phi^2\rangle}{2}e^{-3\alpha}=\langle\hat{H}_m\rangle.$$

We can subtract (6.35) from (6.31) to get

$$i\left(\frac{\partial}{\partial\alpha}-\langle\frac{\partial}{\partial\alpha}\rangle\right)\Psi_\varphi=\sqrt{\frac{3}{\Lambda}}(\hat{H}_m-\langle\hat{H}_m\rangle)\Psi_\varphi+\sqrt{\frac{3}{\Lambda}}\frac{e^{-3\alpha}}{2M^2}\left(\frac{\partial^2}{\partial\alpha^2}-\langle\frac{\partial^2}{\partial\alpha^2}\rangle\right)\Psi_\varphi. \tag{6.36}$$

At leading order, this equation is

$$i\left(\frac{\partial}{\partial\alpha}-\langle\frac{\partial}{\partial\alpha}\rangle\right)\Psi_\varphi=\sqrt{\frac{3}{\Lambda}}(\hat{H}_m-\langle\hat{H}_m\rangle)\Psi_\varphi+O\left(\frac{1}{M_{pl}^2}\right). \tag{6.37}$$

Equation (6.37) is very similar to the results obtained in [22] for the BO approach.

6.3.3 Inner product

Finally, we can take a look at the inner product of our Hilbert space. Equation (6.30) is a Klein-Gordon type equation, so in principle we could take the Klein-Gordon inner product [19] with a suitable prefactor:

$$(\Psi_1, \Psi_2)_{KG} = \int d\phi \sqrt{\frac{3}{\Lambda}} \frac{ie^{-3\alpha}}{M^2} \left(\bar{\Psi}_1 \frac{\partial \Psi_2}{\partial t} - \Psi_2 \frac{\partial \bar{\Psi}_1}{\partial t} \right).$$

We can perform the decomposition

$$\Psi_1 = e^{i\varphi}\Psi_{1,\varphi}, \qquad \Psi_2 = e^{i\varphi}\Psi_{2,\varphi}.$$

We can substitute this in the inner product. After some algebra we obtain:

$$(\Psi_1, \Psi_2)_{KG} = \int d\phi \left[\bar{\Psi}_{1,\varphi}\Psi_{2,\varphi} + \sqrt{\frac{3}{\Lambda}} \frac{ie^{3\alpha}}{2M^2} \left(\bar{\Psi}_{1,\varphi} \frac{\partial \Psi_{1,\varphi}}{\partial t} - \Psi_{2,\varphi} \frac{\partial \bar{\Psi}_{1,\varphi}}{\partial t} \right) \right].$$

We can the see that at leading order the Klein-Gordon inner product is

$$(\Psi_1, \Psi_2)_{KG} = \int d\phi \bar{\Psi}_{1,\varphi}\Psi_{2,\varphi} + O\left(\frac{1}{M^2}\right). \tag{6.38}$$

This is the usual Schrödinger inner product [4].

6.4 Discussion

In the last three subsections we have seen that by including the cosmological constant in our quantum minisuperspace model and choosing the logarithm of the scale factor as our time parameter we can get the result of the Born-Oppenheimer approach before and after quantization [43].

To get it after quantization, we have to perform a phase transformation in the wave function and then ask that the resulting equation is unitary in order to get the Schrödinger equation and the Born-Oppenheimer ansatz. We also saw that the Klein-Gordon inner product reduces to the Schrödinger one if we perform the same phase transformation that we did for the Wheeler-DeWitt equation.

Of course, these results are valid at first order of a series expansion in powers of $\frac{1}{M^2}$. This makes sense, since the results of the Born-Oppenheimer approach are obtained after a series of approximations are considered [4, 6, 11, 22, 43, 45], as we saw in section 6.1.1. Terms of higher order can be considered as corrections to Schrödinger equation coming from quantum gravitational effects [43].

The inclusion of the cosmological constant in the model is fundamental in order to obtain the results we have seen [43]. This arises the natural question if it is possible to obtain the results of the BO approach by choosing a particular gauge in the case in which the cosmological constant is equal to zero. This question is worth exploring and could be a possible extension of this work.

Conclusions

In the present thesis project we studied the problem of time in the context of a quantum FLRW flat spacetime coupled to a scalar field. In chapter five, following the method described in [12], we tried to include time in our formalism by choosing a time parameter as a function of the phase space variables that has Poisson bracket with the Hamiltonian equal to 1. We saw that we can find this time function by solving the equations of motion, applying the constraint, or without applying the constraint.

In particular, in [12], it is argued that in order for the method described to be consistent, the time function should be valid in the whole phase space. However, as we saw in section 5.3, we can still get a consistent quantum theory even if we choose the time function to have Poisson bracket equal to one with the Hamiltonian only in the constraint surface.

Also, the requirement that the time function should be valid in the whole phase space seems to be too restrictive, since in section 5.4, we saw that during the calculations carried out in section 5.2 we had missed a piece of the solution of the canonical transformation we used to go from our old variables to the dynamical ones. This piece was actually fundamental, since the complete result is a Hamiltonian that has a free parameter, which means that the time evolution that we get from the chosen time parameter is not unique.

We attempted to fix this free parameter by comparing the result of the scalar field evolution obtained in the quantum theory with that of the classical theory. We found that we obtain the same result by picking $A = 0$. After picking $A = 0$ the resulting Hamiltonian coincides with the one we got by choosing a time parameter that is valid only on the constraint surface.

Finally, we compare the classical solution we get for the evolution of the scalar field without applying the constraint with the result obtained for the quantum theory, in the hope that they would coincide since the time function was also derived without the application of the constraint. However, we found that they don't coincide even in this case.

On the other hand, in chapter 6, we explored the connection between the Born-Oppenheimer and gauge fixing approaches to the problem of time. We found that if we add a cosmological constant term to our action we can derive the results of the BO approach by choosing α as our time parameter (gauge fixing) [43].

In particular, we saw that this result can be obtained both before and after quantization. To obtain the result after quantization, we should perform a phase transformation in the Wheeler-DeWitt equation where the phase corresponds to the generating function of the change of variables we used in the classical theory.

This work could be further extended by investigating the role of the cosmological constant in the approach. In the work we presented in chapter 6, the addition of the cosmological constant is fundamental to obtain the results, as remarked in [43]. It is worth exploring if there is a gauge fixing that would allow us to obtain the results of the Born-Oppenheimer approach without having to include the cosmological constant.

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