The Wheeler-DeWitt Equation: A Schrödinger Equation for the Origin of the Universe

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Chapter 1

Introduction

The question of the origin of the universe is an ancient one, yet science has had the tools to search for a proper answer for only the last hundred years or so. At that time, though, these tools were neither sufficiently refined nor aimed toward such purpose. Mathematical cosmology is the branch of physics/mathematics currently working on a broad range of subjects including the origin of the universe. Over the last fifty years there has been an increasing interest in solving this particular puzzle [1]. It all started with Einstein's General Relativity.

$$R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R + \Lambda g_{\mu\nu} = \frac{8\pi G}{c^4}T_{\mu\nu}. \tag{1.1}$$

In cosmology one uses this theory to study the universe as a physical system. That is, a system to study mathematically with a set of equations, principles and *sensible* assumptions that agree with observations. Although some models agree to a high degree with current observations, they fail to give a satisfactory answer to the question mentioned. Yet they give several hints that tell us that we should look for the answer within the realm of quantum mechanics. Specifically, we should look for a quantum theory of gravity.

There are many different approaches to quantizing gravity, one of them being

Canonical Quantum Gravity [2]. Each has a different starting point to obtain a quantum theory of gravity. Canonical quantum gravity starts with the tools at hand, namely general relativity and quantum mechanics, and tries to obtain a consistent framework via quantization methods. One of them being the canonical quantization method proposed by Dirac [3], the way QED was achieved. the other is the path integral approach [4]. Both procedures start with the variational principle of general relativity encoded in the action [5]

$$S = \frac{c^4}{16\pi G}\int \sqrt{-g}\,[R-2\Lambda]\,dx^4 + S_{\text{N-G}}, \tag{1.2}$$

where $S_{\text{N-G}}$ represents the Lagrangian density for non-gravitational fields, minimally coupled to gravity (related to $T_{\mu\nu}$ in (1.1)). The former approach, using the ADM formalism (Put forward by R. Arnowitt, S. Deser and C. W. Misner in 1959) obtains a Hamiltonian formulation of general relativity and then uses Dirac's canonical quantization method. The latter approach uses the Feynman path integral formulation with (1.2). With either of these one arrives at the equation

$$\left[\frac{c^8 G_{ijkl}}{(16\pi G)^2}\frac{\delta}{\delta h_{ij}}\frac{\delta}{\delta h_{kl}} + \frac{c^4\sqrt{h}({}^{(3)}R-2\Lambda)}{16\pi G} - T_0^0\right]\Psi\,[h_{ij},\rho] = 0, \tag{1.3}$$

known as the general Wheeler-DeWitt equation. The equation (1.3), derived by Bryce S. DeWitt in 1967 [3], reminds us of the time independent Schrödinger equation $\hat{H}\,|\Psi\rangle = E\,|\Psi\rangle$ for the case $E = 0$. The wave function $\Psi\,[h_{ij},\rho]$ is defined on an infinite-dimensional space of all posible 3-metrics and energy density models, called *superspace* [2]. For cosmology models such as the FRW, it is possible to isolate a finite-dimensional configuration space, the *minisuperspace*, and deduce some properties of $\Psi\,[h_{ij},\rho]$. In this case, the universe is created by means of a tunnelling process which might be related to the inflationary cosmology scenario [6].

The canonical theory of quantum gravity has a lot of problems. Most of them come from the different stages in the derivation of the Wheeler-DeWitt equation. For example, the ADM (1+3) split destroys the four dimensional covariance of general relativity which is not recommended when using Dirac's quantization method. Other problems are related to the factor ordering of the operators and the fact that the mentioned superspace is not a well-behaved Hilbert space [7], and come from the nature of the equation: For non-highly symmetric models the problem of solving (1.3) is virtually impossible [8]. And, finally, since (1.3) inherits its interpretation from quantum mechanics, it is not clear what $\Psi\left[h_{ij}, \rho\right]$ means nor why it is independent of time.

The first attempts to construct a quantum theory of gravity begun in 1930 with the physicist Léon Rosenfeld [10]. In two different papers he traced two different approaches. One would evolve into the *canonical quantization approach* and the other one would evolve into the *covariant quantization approach* [11]. Later, the physicist Matvei Bronstein visualized the problem of the quantization of gravity in the form of a diagram relating the *realms* of physics, namely, classical, relativistic, gravitational and quantum mechanical; known as the Bronstein cube. In that diagram one sees two possible paths to follow to solve the problem: either we quantize gravity directly, that is, to obtain a quantum mechanical equation from Einstein's field equations; or we start with a relativistic quantum field theory and try to connect it somehow with Einstein's field equations. Since quantum mechanics and gravitations were relatively new and not fully understood at that time and because the profound differences between these two theories, these attempts yielded no definite results. The subject lost momentum until 1950, when people were again greatly interested in obtaining a quantum theory of gravity.

In the mid 50's, John Wheeler and his student Charles Misner, making parallels between QED and gravity in geometrical concepts and applying quantum mechanical ideas to the space-time at small scales, conceived a theory called *quantum geometrodynamics* [12]. It supposed a basis for the search of a quantum theory of gravity. Later, Misner suggested three lines of research in quantum gravity, one of them consisted of rewriting general relativity using Dirac's constrained Hamiltonian formulation and then using a quantization method developed by Peter Bergman. This is the spirit of the canonical approach. In 1961, the physicists Charles Misner, Richard Arnowitt and Stanley Deser, published the constrained Hamiltonian formulation of general relativity known as the ADM formalism [13]. In 1965 Wheeler and the physicist Bryce DeWitt started discussing the recently developed ADM formalism and thought about doing for relativity what Schrödinger had done for the hydrogen atom in 1925 [10]. The result of these conversations was a series of papers published in 1967 that described the canonical approach to quantum gravity [3]. Equation (1.3) made its first appearance in physics. Shortly after deriving it, DeWitt realized there were a lot of problems of this equation. Some of them we've already mentioned. These problems kept it from being considered a full theory of quantum gravity, but the attempts to solve some of them have led to different and also promising theories. For example, loop quantum gravity through the Ashtekar variables representation of general relativity. Nowadays the Weeler-DeWitt equation is just one of several lines of research in the path to understand gravity at a quantum level, yet it is considered to be the beginning of formal attempts to construct a theory of quantum cosmology and it is still a prevalent subject [14].

We plan to review and study in detail the canonical quantum gravity programme, whose problems and consequences are still to be thoroughly revised in the aim of obtaining a quantum theory of gravity.

Chapter 2

Classical Cosmology

Cosmology is the study of the universe and all that it contains and tries to explain how does it evolve or work as a whole. In that sense, it is a very old subject. It goes back thousands of years to any culture that tried to understand the world around them. Of course these ideas evolved with time and now, what we call the modern subject of cosmology (the science of cosmology), is relatively new. Its origin can be traced back to somewhere between the second quarter of the 20^{th} century, when Eddwin Hubble discovered that the universe is expanding, and the discovery of the 2.72k CMB radiation, as a remanent of the Big Bang, in the 60's. Before that cosmology was less like physics and more like a *natural science*.

Cosmology is now a branch of physics and as such it is the study of the universe as a physical system. That is, a system to study mathematically with a set of equations, principles and *sensible* assumptions that agree with observations. Different assumptions give rise different cosmological models but the one we are interested in is the Friedmann-Robertson-Walker model. The Friedmann equation is one of the most important equations in modern cosmology since it describes the evolution of *our* universe. In this chapter we are going to derive it within the theory of general relativity and discuss some of its solutions.

2.1 The Friedmann Equations

2.1.1 Derivation

The main idea of the derivation in this section is to use some assumptions to find a convenient form for the metric tensor and the energy-momentum tensor, and then use Einstein's field equation[1]. The derivation of the Friedmann equation, and, in fact, most of modern cosmology, is based en the **Cosmological Principle**. It states that the universe is isotropic and homogeneous in large enough scales. In small scales this is not true: if you look towards the sun, the universe would look different than if you look away from it. Large enough scales mean 10^8 light-years and larger [12]. The cosmological principle relies on astronomical observations[2]; the universe looks isotropic from our point of view and unless we happen to be in a very special place in it, we should believe that it is homogeneous; so isotropy around every point implies homogeneity. In other words the cosmological principle says that the universe is the same everywhere and looks the same in every direction and there is no "especial" or preferred place in it [5]. It is evident though, that the universe evolves in time and we can distinguish between past, present and future. Then the cosmological principle applies only to the space part of the space-time. This fact allows us to write the space-time metric as

$$ds^2 = -dt^2 + a^2(t)h_{ij}dx^i dx^j. \tag{2.1}$$

Here t is the time coordinate and (x^1, x^2, x^3) are the coordinates of the sub-manifold (space) Σ of the space-time $\mathbb{R}\times\Sigma$. Note that the coordinates we use in (2.1) allows let us write the metric without crossed terms $dtdx^i$ and that the coefficient for dt^2 is independent of the x^i's. These coordinates are known as the

[1]Throughout this chapter we are going to set $c = 1$

[2]The Cosmological Principle, in reality, has a status somewhere between being a postulate (and therefore highly questionable) and an observational fact. In some scales it looks homogeneous and isotropic but, in scales so big that we can't see them, we really don't know if that is true. [16] [17] [18] [19] [20].

comoving coordinates and are the ones that are carried along with the expansion. $a(t)$ is the scale factor and is responsible for keeping track of how big or small is the universe at some time t.

These ideas of *same everywhere and in every direction* are closely related to the concept of isometry. Since in our universe we measure distances using a metric, it is somewhat natural to think that isotropy and homogeneity mean that the metric should *behave* the same at every point. Mathematically speaking, a manifold is homogeneous around a point p if there is a infinitesimal homogeneous that maps p into another point q in its neighbourhood, and it is isotropic if for every pair of tangent vectors v and w at p there is an infinitesimal isometry that maps p into himself and maps v into w [21]. These infinitesimal isometries are also called Killing vectors [22]. The cosmological principle implies that the space part of the universe must have the maximum number of independent Killing vectors $n(n+1)/2$, that is, it must be a maximally symmetric manifold. With this, the cosmological principle becomes a purely geometrical statement!. For a maximally symmetric manifold of dimension n, the Riemannian curvature tensor obeys the equation

$$R_{\rho\sigma\mu\nu} = \kappa \left(g_{\rho\mu} g_{\sigma\nu} - g_{\rho\nu} g_{\sigma\mu} \right).$$

Where κ is a constant proportional to the scalar curvature R.

$$\kappa = \frac{R}{n(n-1)}.$$

We should remember that up to these point we are talking only about Σ, so we are calculating these quantities in a $n = 3$ manifold. Then, the relations [1]

$$R_{ijkl} = \kappa \left(h_{ik} h_{jl} - h_{il} h_{jk} \right) \tag{2.2}$$

[1] It is a convention in general relativity to use Greek indices yet here we changed them to Latin ones to remember that we are talking about Σ and not the space-time itself.

and

$$\kappa = R/6 \tag{2.3}$$

hold. By contracting indices i and k we get the Ricci curvature tensor

$$R_{jl} = 2\kappa h_{jl}. \tag{2.4}$$

It shouldn't come as a surprise that the scalar curvature of Σ is constant. If it weren't our universe would have some sort of "lumps" and we would be able to see them by measuring densities at different places. The maximally symmetric property of Σ enables us to write h_{ij} as[1]

$$h_{ij}dx^i dx^j = e^{2\beta(r)}dr^2 + r^2 d\Omega^2, \tag{2.5}$$

in spherical coordinates. r is the radial component and $d\Omega^2$ the metric of $\mathbb{S}^2$. At this point we can calculate the components of the Ricci tensor

$$\begin{aligned} R_{11} &= \frac{2}{r}\partial_1\beta \\ R_{22} &= e^{-2\beta}(r\partial_1 - 1) + 1 \\ R_{33} &= R_{22}\sin^2(\theta). \end{aligned} \tag{2.6}$$

Using the equation (2.4) we find an expression for $\beta(r)$

$$\beta(r) = -\frac{1}{2}\ln(1 - \kappa r^2), \tag{2.7}$$

and, finally

$$ds^2 = -dt^2 + a^2(t)\left(\frac{dr^2}{1 - \kappa r^2} + r^2 d\Omega^2\right) \tag{2.8}$$

[1]A complete explanation of why this is possible can be found in [21]. This is related to the fact that Killing vectors are symmetry generators.

Equation (2.8) is known as **Robertson-Walker (RW)** metric. If we consider the transformation

$$\begin{aligned} \kappa &\to \hat{\kappa} = \frac{\kappa}{|\kappa|} \\ r &\to \hat{r} = \sqrt{|\kappa|}r \\ a &\to \hat{a} = \frac{a}{\sqrt{|\kappa|}} \end{aligned} \tag{2.9}$$

we see that

$$\begin{aligned} d\hat{s}^2 &= -dt^2 + \hat{a}^2(t)\left(\frac{d\hat{r}^2}{1-\hat{\kappa}\hat{r}^2} + \hat{r}^2 d\Omega^2\right) \\ &= -dt^2 + \frac{a^2(t)}{|\kappa|}\left(\frac{|\kappa|dr^2}{1-\frac{\kappa}{|\kappa|}|\kappa|r^2} + |\kappa|r^2 d\Omega^2\right) \\ &= ds^2, \end{aligned}$$

then the metric is invariant under the transformation. In other words, if we multiply the metric by a constant, by (2.4), we see that the curvature is divided by the same constant. κ is the only relevant parameter and there are three different cases: $\kappa \in \{-1, 0, 1\}$. So there are only tree classes of homogeneous and isotropic manifolds, namely the hyperbolic space $\mathbb{H}^n$ (negative curvature), the flat space $\mathbb{R}^n$ (zero curvature) and the n-sphere $\mathbb{S}^n$ (positive curvature)[1]. Formally, if a manifold has constant curvature, its universal covering is isometric to one of these spaces [22]. The torus is a special case of a manifold with constant curvature. It is actually flat but with periodic conditions at the boundaries and it is not a popular idea to think about the universe in that way. Before proceeding lets define $\dot{a} \equiv \frac{da}{dt}$. Now that we have the metric we can calculate the Riemannian

[1]In [12] the reader can find cosmological models that don't assume the cosmological principle.

connection coefficients

$$\begin{aligned}
\Gamma^0_{11} &= \frac{a\dot{a}}{1-\kappa r^2} \quad \Gamma^0_{22} = a\dot{a}r^2 \quad \Gamma^0_{33} = \Gamma^0_{22}\sin^2\theta \\
\Gamma^1_{01} &= \Gamma^2_{02} = \Gamma^3_{03} = \frac{\dot{a}}{a} \\
\Gamma^1_{22} &= -r\left(1-\kappa r^2\right) \quad \Gamma^1_{33} = \Gamma^1_{22}\sin^2\theta \\
\Gamma^2_{12} &= \Gamma^3_{13} = \frac{1}{r} \\
\Gamma^2_{33} &= -\sin\theta\cos\theta \quad \Gamma^3_{23} = \cot\theta.
\end{aligned} \tag{2.10}$$

the components of the Ricci tensor are

$$\begin{aligned}
R_{00} &= -\frac{\ddot{a}}{a} \\
R_{11} &= \frac{a\ddot{a}+2a^2+2\kappa}{1-\kappa r^2} \\
R_{22} &= r^2(a\ddot{a}+2a^2+2\kappa) \\
R_{33} &= R_{22}\sin^2\theta
\end{aligned} \tag{2.11}$$

and the scalar curvature is

$$R = 6\left[\frac{\ddot{a}}{a} + \left(\frac{\dot{a}}{a}\right)^2 + \frac{\kappa}{a^2}\right]. \tag{2.12}$$

With this we have completely determined the purely geometric part of Einstein's filed equation. Since the universe is not empty, the next step is to mathematically model its content. This is achieved by choosing an appropriate energy-momentum tensor $T_{\mu\nu}$. At large scales we can think of galaxies become as non-interacting "particles", More precisely, averaging over large scales the content of the universe becomes a perfect fluid, and in the same sense that we describe a particle by a 4-momentum $p^\mu = (E, p_1, p_2, p_3)$, we describe the fluid by[1].

$$T_{\mu\nu} = (\rho + p)U_\mu U_\nu + p g_{\mu\nu}. \tag{2.13}$$

ρ and p are the energy density and the pressure of the fluid, respectively. $U_\mu = (1, 0, 0, 0)$ is the 4-velocity of the fluid in the comoving coordinates, i.e., the coordinates we need to be to see the homogeneity and isotropy of the universe. We can think of it as if the particles are embedded or glued to a "grid", so if the the grid changes the fluid changes accordingly. The case for which the change is an expansion is represented in figure 2.1.

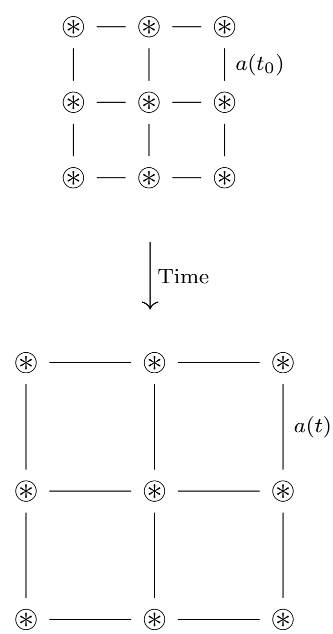

Figure 2.1: Expansion of the universe. The grid represents a coordinate system. Since space is isotropic and homogeneous, the important parameter is represented by $a(t)$

[1]In [23] there is a nice summary about how to interpret $T_{\mu\nu}$

Plugging the 4-velocity in (2.13) we get

$$T^{\mu}_{\nu} = \begin{pmatrix} -\rho & 0 & 0 & 0 \\ 0 & p & 0 & 0 \\ 0 & 0 & p & 0 \\ 0 & 0 & 0 & p \end{pmatrix}. \tag{2.14}$$

If we include the cosmological constant[1] Λ, Einstein's equation becomes

$$G_{\mu\nu} = 8\pi G T_{\mu\nu} - \Lambda g_{\mu\nu}. \tag{2.15}$$

Equation (2.15) becomes

$$G_{\mu\nu} = \begin{pmatrix} 8\pi G\rho + \Lambda & 0 & 0 & 0 \\ 0 & -8\pi G p + \Lambda & 0 & 0 \\ 0 & 0 & -8\pi G p + \Lambda & 0 \\ 0 & 0 & 0 & -8\pi G p + \Lambda \end{pmatrix}. \tag{2.16}$$

On the other hand, unsing equations (2.8), (2.11) and (2.12) we obtain

$$G_{00} = 3\left(\frac{\dot{a}}{a}\right)^2 + \frac{3\kappa}{a^2} \tag{2.17}$$

and

$$G_{ii} = -2\frac{\ddot{a}}{a} - \left(\frac{\dot{a}}{a}\right)^2 - \frac{\kappa}{a^2}, \quad i \in \{1, 2, 3\} \tag{2.18}$$

The other components are vanish ($G_{\mu\nu} = 0,\ \ \mu \neq \nu$). Equating each component in (2.16), (2.17) and (2.18) we get

[1] We are going include Λ in our derivation of Friedmann equations and the next section we are shall explain its significance.

$$\left(\frac{\dot{a}}{a}\right)^2 = -\frac{\kappa}{a^2} + \frac{\Lambda}{3} + \frac{8\pi G}{3}\rho \tag{2.19}$$

and

$$\begin{aligned} 2\frac{\ddot{a}}{a} &= -\left(\frac{\dot{a}}{a}\right)^2 - \frac{\kappa}{a^2} + \Lambda - 8\pi G p \\ &= -\frac{8\pi G}{3}(\rho + 3p) + \frac{2\Lambda}{3} \end{aligned} \tag{2.20}$$

Equation (2.19) is known as **the Friedmann equation** and (2.20) is called **the second Friedmann equation**. These equation together with the metric (2.8) are knwn as the **Friedmann-Robertson-Walker model (FRW)**. We should remember that a has no physical meaning up to this point. Recalling the figure in page 11 if we ask ourselves how big is a, the answer is: it depends. It depends on the grid we have laid down on space, so a is really a bookkeeping device and doesn't mean anything by itself. On the other hand, ratios of a may mean something. If we change a by $a' = 3a$ (the physical distance between every pair of points in the universe triples) we clearly get $\dot{a}' = 2\dot{a}$ and

$$\frac{\dot{a}}{a} = \frac{\dot{a}'}{a'}. \tag{2.21}$$

So ratios of a don't depend on the grid and they can be interpreted. Equation (2.21) is so important that it gets its own name: **Hubble parameter** H.

$$H \equiv \frac{\dot{a}}{a} \tag{2.22}$$

and the Friedmann equations can be rewritten as

$$H^2 = -\frac{\kappa}{a^2} + \frac{\Lambda}{3} + \frac{8\pi G}{3}\rho \tag{2.23}$$

We have derived the Friedmann equations using general relativity but it is possible to do the same thing using Newton's laws and the first law of thermodynamics [24] [25]. As a consequence it is possible to make an analogy between an expanding or contracting universe and the problem of a particle that is trying to escape a gravitational field. The equations obtained by Newton's laws are identical to (2.19) and (2.20) except for the cosmological constant factor[1]. This is not a strange result. Even if our universe is curved, if we look at very neighbouring galaxies (local behaviour of the universe) we shouldn't worry about the fact that the universe has curvature and this is completely consistent with general relativity. We could run into trouble though, if the galaxies or particles are moving relative to each other with a significant fraction of c. But there are particles moving with such speed! (photons). The universe is filled with homogeneous radiation. This means that the equations have to be modified to account for this form of energy. In the next section we shall mention this.

2.2 Different universes at different times

To study the solutions to (2.19), we first must find the fluid equation, i.e., a relation between ρ, p and a. This can be achieved using energy conservation principle $\nabla_\mu T^{\mu\nu} = 0$ [21].

$$0 = \nabla_\mu T^\mu_0 = -\dot{\rho} - 3\frac{\dot{a}}{a}(\rho + p). \tag{2.24}$$

There are two paths we can follow. Either we choose a general equation of state for the content of the universe (a relation between ρ and p in the same sense as in thermodynamics) or we can analyse what ρ would be for each source of energy independently and solve (2.19). We shall follow the latter since it gives a better insight about the relation between space and its content. For simplicity,

[1] It is possible to find an analogous to the cosmological constant in Newton's gravitational law [26].

we are going to concentrate in one term of the right hand side of (2.19) at a time and ignore the rest; later we shall talk about the full equation. So, What does the universe has in it? Obviously enough, it has non-relativistic matter. This is the first case.

2.2.1 Matter dominated universe

Here we imagine the universe to be filled only with non-relativistic particles (that's the reason it is called matter dominated. For a simple gas we know that the bigger the energy, the bigger the pressure; but this energy is related to the velocity of the particles. When we say that the particles are non-relativistic we mean that the particles are practically at rest and the contribution to the energy density comes only from $E = mc^2$ and the gas exerts no pressure on the walls of the box. So we take $p = 0$ and plug it in (2.24) to get

$$\rho = \frac{\rho_0}{a^3}. \tag{2.25}$$

If we think about a box filled with non-relativistic particles (i.e. Mass times velocity squared $\ll$ than mc^2) and then imagine that we stretch the box, it is not hard to see that the energy density would fall as a^{-3}. The energy is spread over a larger volume. ρ_0 is a tunable factor and can be determined from the initial conditions of the differential equation. Putting (2.25) into (2.23) gives

$$a(t) = \left(\frac{t}{t_0}\right)^{2/3}. \tag{2.26}$$

t_0, as ρ_0, is a tunable parameter fixed only by the initial conditions. Equation (2.26) states that the universe is growing but the rate at which it grows decreases with time, i.e., it is decelerating, yet gravity never overcomes the expansion and it will never come to a stop or re-collapse. This is evident in figure 2.2. Another interesting feature is that $a(t = 0) = 0$, so the universe start from a point (singularity). Now lets consider the case where the universe has only radiation in it.

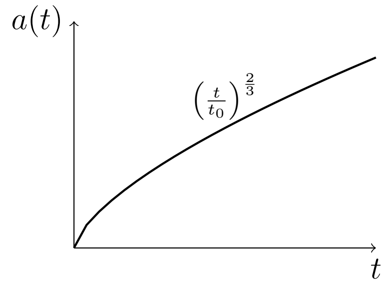

Figure 2.2: Matter dominated universe.

2.2.2 Radiation dominated universe

This case is rather similar to the matter dominated universe. The mental picture used there also works here but we must make a little change. The box is now filled with photons. Clearly the photon density falls as a^{-3}, but the energy density falls as a^{-4}. To understand this imagine a photon inside a box. If we stretch the box, the wavelength would expand too[1] with a. Since the energy of a photon is $E = hc/\lambda$, for every photon in the box there is a loss of energy proportional to a^{-1} (cosmological redshift). This loss of energy is equal to the work done on the "walls" of the universe to expand it.

$$\rho = \frac{\rho_0}{a^4}. \tag{2.27}$$

Putting the equation of state for radiation, $p = \rho/3$, into (2.24), yields the same result. The equation of state can be derived by proving that the electromagnetic tensor is traceless and equating it to the trace of energy-momentum tensor [2]. An heuristic argument can also be used [24]. Using (2.27) and the Friedmann equation gives

[1]The reason why as the universe expands the wavelength of a photon would match it is that the number of nodes of a wave is an adiabatic invariant

$$a(t) = \left(\frac{t}{t_0}\right)^{1/2}. \tag{2.28}$$

Same as before, the radiation dominated universe start out as a single point and grows forever with an ever decelerating expansion $H = 1/2t$, yet the rate of expansion is slower. In figure 2.3 we find the comparison between the two universes.

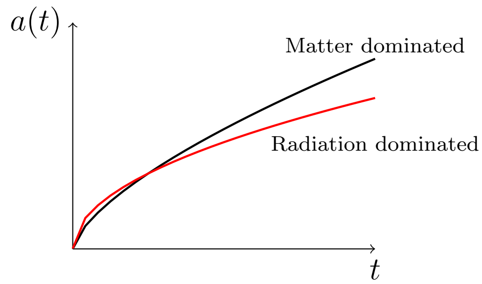

Figure 2.3: Radiation dominated (red) Vs. a Matter dominated universe (black).

2.2.3 Curvature

Lets examine what happens when we consider, both, curvature κ and energy density ρ. We can write (2.19) as

$$\left(\frac{\dot{a}}{a}\right)^2 = -\frac{\kappa}{a^2} + \frac{8\pi G}{3}\rho. \tag{2.29}$$

For every possible value of κ we get different behaviours. Clearly, if $\kappa = 0$ (flat space) we obtain a matter dominated or radiation dominated universe, depending on what replaces ρ. On the other hand, if $\kappa = -1$, the right hand side of (2.29) is always positive. This means that $\dot{a}$ never changes sign. Since we know that the universe is expanding, $\dot{a}$ must be positive and we get an ever expanding universe with a singularity as the origin. Assuming that $\dot{a}$ is negative would give you an ever shrinking universe (not a very realistic case). Finally, if $\kappa = +1$, we get an expanding universe that stops at some value a and then starts shrinking until it collapses into a singularity. To see this, remember that the matter energy density and the radiation energy density decays as a^{-3} and a^{-4} respectively. So the density term will be less than 1 for some time t. But this can't happen since the left hand side of (2.29) is squared. Then, a can't grow without bounds. It must get to a maximum value and it should star decreasing after that. The comparison appear in figure 2.4.

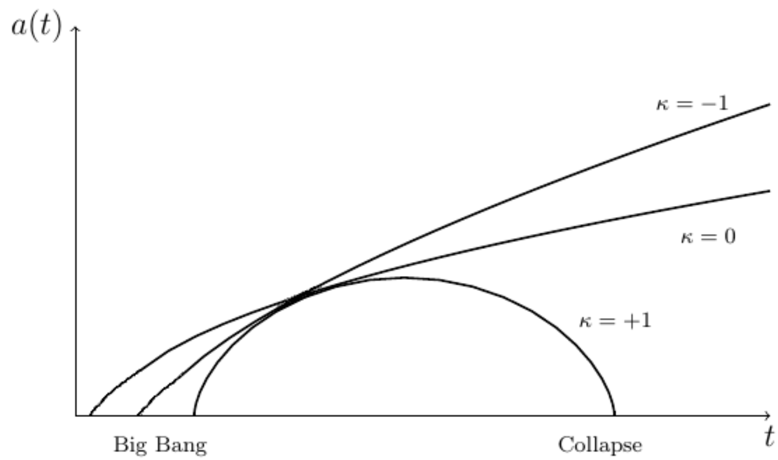

Figure 2.4: Evolution of a for the different values of κ

It is also possible to ignore the energy density of matter and radiation altogether. In this case, the resulting universe consists of the limiting case between a decelerating universe and an accelerating one, i.e, a obeys the equation

$$a(t) = \frac{t}{t_0}. \tag{2.30}$$

This universe grows forever but at a constant rate.

2.2.4 Vacuum dominated universe

Lastly, we consider a universe in which only the cosmological constant is important. By inpecting (2.15) we can see that Λ corresponds to a perfect fluid with the characteristic that its state equation is $p = \rho$. How odd is that? Our image of a box with particles is useless, yet there is a somewhat familiar example of such behaviour. Replace the box by a string with the ends joined by a spring. This system has the property that the pressure is negative (tension of the string) if the energy density (potential energy of the spring) is positive. The more energy the spring has, the more negative is the pressure. The energy density of Λ is $\rho = \Lambda/8\pi G$. The fact that is constant means that empty space does not dilute as it expands. Solving Friedman equation yields

$$a(t) = a_0 \exp\left[\sqrt{\frac{\Lambda}{3}}t\right]. \tag{2.31}$$

Under these conditions, the scale factor does not behaves as a polynomial but as an exponential function.

2.2.5 Mixtures

At every step of this section we have purposely ignored different terms of the Friedmann equation in order to obtain simple solution for the evolution of a. Of course, the universe is not that simple. In the general case (the realistic case), we should take into account every contribution for (2.19). The exercise is not completely futile. Everything we have said about the energy densities is true, that is, they do have the a dependence we stated ($\rho_{\text{matter}} \propto a^{-3}$, $\rho_{\text{radiation}} \propto a^{-4}$, $\rho_{\text{curvature}} \propto a^{-2}$ and $\rho_\Lambda = \Lambda/8\pi G$). Then it is easy to see that the cosmological constant is more important for $t \to \infty$, the curvature dominates the universe at $t \to 0$, and at intermediate times, the universe is matter dominated and radiation dominated. So, by fixing the values of the constants, it is possible to study the universe (at different times) with a high degree of realism.

2.3 Inflation

Now that we have discussed the general picture of classical cosmology, it is time to mention some of it shortcomings. As we have mention, the FRW model is based on the observation that the universe is isotropic and homogeneous. However it does not tell us why the universe is that way. The microwave background radiation is evidence that the universe is quite isotropic since, to a great accuracy, it has the same temperature ($2.725K$) in all regions of the sky. The problem is that radiation we receive from opposite sides of the sky has been travelling towards us since decoupling so, the two regions on opposite sides haven't had the time to interact in some way. Hence, no thermal equilibrium can be achieved. On the other hand, The microwave background is not perfectly isotropic, but instead it has some small fluctuations. These irregularities are thought to represent the *seeds* from which structure like stars, galaxies, clusters and voids come to be. Standard cosmology does not explain the origin of such fluctuations. These problems are known as the horizon problem and the small scale inhomogeneities.

Another issue that haunts classical cosmology is the flatness problem. The Fiedmann equation can be rewritten using the total density of material Ω_{tot} as

$$|\Omega_{tot} - 1| = \frac{\kappa}{a^2 H^2}. \tag{2.32}$$

From this we see that if the total density is equal to one, the it remains so for all time. However, if it is not one, from the discussion we made for matter dominated or radiation dominated universes, it would evolve as

$$|\Omega_{tot} - 1| \propto t^{2/3}. \tag{2.33}$$

or

$$|\Omega_{tot} - 1| \propto t. \tag{2.34}$$

respectively. This means that an universe with a flat geometry is unstable. Any deviation from flatness would rapidly evolve into a more and more curved universe. The problem is that it is known that the density parameter lies between 0.5 and 1.5, which implies that the early universe must have been incredibly close to flat [24]. Again, classical does not explain why.

Alan Guth proposed the inflationary expansion as a solution to these problems. He defined it as a period in the evolution of the universe during which the scale factor rapidly grows $\ddot{a} > 0$. As we have seen, a dramatic growth of the scale factor is possible for vacuum dominated universes. Using equation (2.35) we can rewrite equation (2.34) as

$$|\Omega_{tot} - 1| = \exp\left[-\sqrt{\frac{4\Lambda}{3}}t\right]. \tag{2.35}$$

Hence, a vacuum dominated universe *forces* flatness. The inflationary scenario also fixes the horizon problem and the small scale inhomogeneities. Inflation greatly increases the size of a region of the universe while keeping its characteristic scale. This means that a region of the universe small enough to achieve thermal equilibrium expands to be much larger than the observable universe. By this, we can say that the microwaves from opposite sides of the universe are at the same temperature because they were once in equilibrium.

Chapter 3

The Wheeler-DeWitt Equation

In this chapter, we will concern ourselves with the derivation of the general Wheeler-DeWitt equation. As we mentioned before, as an attempt to obtain a quantum theory of gravity, such equation comes from applying Dirac's quantization technique to the general relativity Hamiltonian. Then, the road to the Wheeler-DeWitt equation, which we will follow here, consists of two main steps: First, we will obtain the Hamiltonain from the Hilbert-Einstein action. Then we will use Dirac's method to obtain equation (1.3).

Finally, to link to our previous chapter, we will use the FRW model as an example of the an application of the Wheeler-DeWitt equation.

3.1 The ADM Formalism

One of the most widely used Hamiltonian formulations of General relativity is the ADM formalism was developed by R. Arnowitt, S. Deser, and C. W. Misner [27] in 1962. The main idea behind such formalism is to ignore the notion of time as just another coordinate in space-time and develop the theory in a way which separates time coordinate [28]. This is generally known as the $(1 + 3)$ form of the theory. The outline of the formulation is as follows: First, we split the space-time into a series of space-like hyper-surfaces parametrized by a vector field $\partial_\mu t$. Then, we use a congruence of curves to provide the space-time and the hyper-surfaces with a natural set of coordinates[1]. Once we have our set of coordinates we note that the 4-metric splits into normal and tangent components to the space-like hyper-surfaces. In such splitting, the 4-metric can be re-expressed in terms of the induced 3-metric h_{ij} and four functions N and N^i. Then we rewrite the Lagrangian in terms of these variables and treat them as conjugate variables of the action principle. When the conjugate momenta to the three conjugate variables we observe that the conjugate momenta to N and N^i vanish. This means that N and N^i are not true degrees of freedom and should be treated as Lagrange multipliers. Varying the action with respect to N and N^i we obtain two constraint equations. And finally, putting everything back together we obtain a constrained Hamiltonian formulation of general relativity.

3.1.1 1+3 Split

Our objective is to obtain the Hamiltonian from the action

$$S = \int \sqrt{-g}\frac{c^4}{16\pi G}\left[R - 2\Lambda\right] dx^4 + S_{\text{N-G}}. \tag{3.1}$$

In the Hamiltonian formulation of a classical theory, first we construct a Lagrangian $\mathcal{L}$ by examining the system we wish to study. The $\mathcal{L}$ is expressed in terms of generalized coordinates q and $\dot{q}$. In our case, the dynamical variables are the components of the metric tensor[2] $g_{\mu\nu}$. Once we have the Lagrangian, the canonical momenta is defined as:

$$p = \frac{\partial \mathcal{L}}{\partial \dot{q}}, \tag{3.2}$$

and the Hamiltonian density is $\mathcal{H} \equiv \sum pq - \mathcal{L}$. In the case of general relativity,

[1]This first two steps are the foliation of space-time

[2]Throughout this chapter we will use Greek indices for 4-dimensional quantities $(0, 1, 2, 3)$ and Latin indices for 3-dimensional quantities $(1, 2, 3)$

our case, the Hamiltonian is

$$\mathcal{H} = p^{\mu\nu} g_{\mu\nu} - \mathcal{L}. \tag{3.3}$$

where the $\dot{g}_{\mu\nu}$'s are expressed as functions of the $p^{\mu\nu}$'s. $\mathcal{H}$ is thus expressed in terms of generalized coordinates $g_{\mu\nu}$ and canonical momenta $p^{\mu\nu}$. The procedure displayed in equations (3.2) and (3.3) was the one used by Dirac [29], but we are going to follow a different approach in which we change the representation of the dynamical variable by splitting the space-time manifold into space and time [30]. First, we assume that the space-time $(\mathcal{M}, g)$ is globally hyperbolic and posses a topology of $\Sigma \times \mathbb{R}$. This allows us to foliate $\mathcal{M}$ as a set of non-intersecting space-like hyper-surfaces. Such hyper-surfaces are defined by a scalar field $t(x^\mu)$ such that t =constant. The vector field

$$\zeta_\mu = \nabla_\mu t = \partial_\mu t \tag{3.4}$$

will be normal to the hyper-surfaces Σ_t for each value of t. In each hyper-surface we can stablish a set of coordinates y^i. Now, we want define a coordinate system to label the events on $\mathcal{M}$ using y^i. For this, we must find a relation between the coordinates systems of Σ_t for two different values t_1 and t_2.

Consider a congruence of curves that intersect Σ_{t_1} and Σ_{t_2}. For a single curve γ, using t as the curve parameter, we can define a map between events $P_t \in \Sigma_t$ as in figure 3.1. Such map allows us make the coordinates y^i constant on each curve by imposing the condition $y^i(P_{t_1}) = y^i(P_{t_2})$. With this, we can label the events on $\mathcal{M}$ by the coordinate system $x^\mu = (t, y^i)$, called the *adapted* coordinate system. Clearly, by construction, the vector field $t^\mu = \partial x^\mu / \partial t$ is tangent to each curve in the congruence and satisfies the condition

$$\zeta_\mu t^\mu = 1. \tag{3.5}$$

The relation between the coordinate system x^μ and y^i is given by the matrix

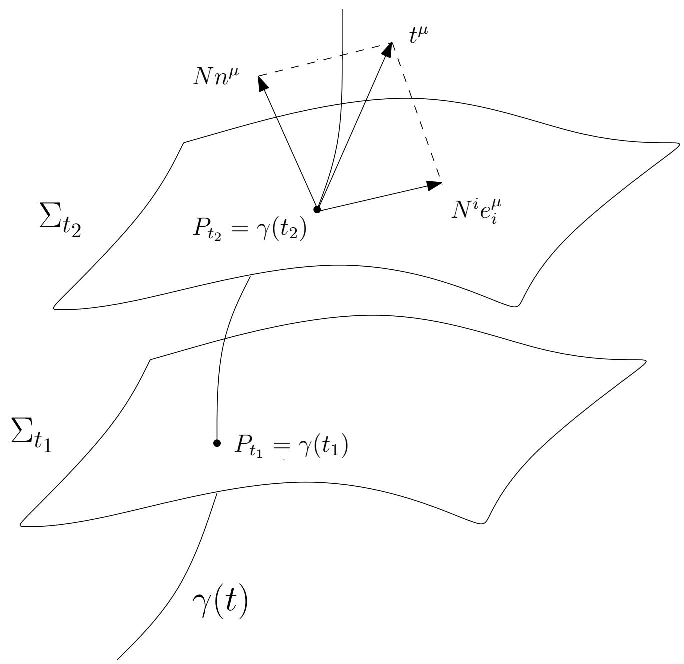

Figure 3.1: Foliation of $\mathcal{M}$.

$$e_i^\mu = \frac{\partial x^\mu}{\partial y^i}, \tag{3.6}$$

also known as the projection tetrad [31]. By construction, the vectors e_i^μ for each i form a basis for Σ and can be used to project any 4-dimensional tensorial quantity $T_{ij\ldots} = T_{\mu\nu\ldots} e_i^\mu e_j^\nu \ldots$. They are 4-vectors because we are considering the hyper-surface as embedded in the ambient space $\mathcal{M}$. Since we have $\zeta_\mu e_i^\mu = 0$, ζ_μ and e_i^μ form a basis for $\mathcal{M}$. At this point we introduce four functions which are related to the projection of the vector t^μ onto the mentioned basis. The first one, called the **lapse** function N, is defined as scalar factor of the vector ζ_μ such that if

$$n^\mu = \frac{\zeta^\mu}{|\zeta^\mu \zeta_\mu|^{1/2}}, \tag{3.7}$$

then the following equation holds

$$N = n^\mu t_\mu. \tag{3.8}$$

The other three functions form a 3-vector N^i called the **shift** vector and each component is defined as the coefficient of the projection of t^μ onto Σ. Then we have

$$t^\mu = N n^\mu + N^i e_i^\mu. \tag{3.9}$$

Using the coordinate transformation $x^\mu = x^\mu(t, y^i)$ and equations (3.4), (3.6) and (3.9) we can write the differential

$$\begin{aligned} dx^\mu &= \frac{\partial x^\mu}{\partial t} dt + \frac{\partial x^\mu}{\partial y^i} dy^i \qquad (3.10) \\ &= t^\mu dt + e_i^\mu dy^i \\ &= (N n^\mu + N^i e_i^\mu) dt + e_i^\mu dy^i \qquad (3.11) \end{aligned}$$

Everything we have done up until now is so we can rewrite the metric tensor $g_{\mu\nu}$ in terms of different variables: the lapse function, the shift vector and the **induced 3-metric**

$$h_{ij} = g_{\mu\nu} e^\mu_i e^\nu_j. \tag{3.12}$$

To achieve this, we calculate the line element using equation (3.10).

$$\begin{aligned} ds^2 &= dx^\mu dx_\mu \\ &= ((Nn^\mu + N^i e^\mu_i)dt + e^\mu_i dy^i)((Nn_\mu + N^i e_{\mu i})dt + e_{\mu i} dy^i) \\ &= ((Nn^\mu + N^i e^\mu_i)dt + e^\mu_i dy^i) g_{\mu\nu} ((Nn^\mu + N^j e^\mu_j)dt + e^\mu_j dy^j) \\ &= (-N^2 + h_{ij} N^i N^j) dt^2 + h_{ij} dy^i dy^j + 2h_{ij} N^i dy^j dt \\ &= -N^2 dt^2 + h_{ij}(dx^i + N^i dt)(dx^j + N^j dt) \end{aligned} \tag{3.13}$$

With this result we can find the desired expressions for the different components of the metric tensor in terms of our new variables

$$g_{\mu\nu} = \left(\begin{array}{c|c} -N^2 + N_i N^i & N_j \\ \hline N_i & h_{ij} \end{array}\right), \tag{3.14}$$

with inverse

$$g^{\mu\nu} = \left(\begin{array}{c|c} -N^{-2} & N^{-2} N^i \\ \hline N^{-2} N^j & h^{ij} - N^{-2} N^i N^j \end{array}\right). \tag{3.15}$$

This also shows that the variables N, N_i and h_{ij} contain the same information as $g_{\mu\nu}$. Thus, rewriting the Lagrangian given above in terms of these variables is completely valid step. From linear algebra we know that for an invertible matrix A it holds that $A^{-1} = \frac{1}{\det A} C^T$ where C is the cofactor matrix. In particular, we get the relation $g^{00} = \text{cofactor}(g_{00})/g = (-1)^2 h/g$. Using (3.14) and (3.15), it follows that

$$\sqrt{-g} = N\sqrt{h}. \tag{3.16}$$

Equations (3.9), (3.14), and (3.16) are the main results of the $1+3$ split of the space-time manifold which was achieved by foliating $\mathcal{M}$ by space-like hyper-surfaces Σ_t. Before rewriting the Lagrangian, we will need to introduce some structures and equations related to the geometry of the space-like hyper-surfaces.

3.1.2 Intrinsic Derivative, Extrinsic Curvature and Riemann Tensor

Now that we have foliated $\mathcal{M}$, we are going to cover some properties of space-like hyper-surfaces that will be useful when trying to apply the change of variables to the Hilbert-Einstein action. The main terms in it are $\sqrt{-g}$ an R. We already calculated $\sqrt{-g}$ in equation (3.16). Hence our main mission is to find an expression for R. First lets note that the 3-metric can be expressed in a 4-dimensional form [32]

$$h^{\mu\nu} \equiv h^{ij} e_i^\mu e_j^\nu = g^{\mu\nu} + n^\mu n^\nu. \tag{3.17}$$

The right hand side of the equation can be interpreted as coming from the Gram-Schmidt process since, for a general vector field, the projection means subtracting the component on the n^μ direction. That is

$$\begin{aligned} V^\nu + n^\nu g_{\mu\alpha} n^\mu V^\alpha &= g^{\mu\nu} V_\mu + n^\mu n^\nu V_\mu \\ &= (g^{\mu\nu} + n^\mu n^\nu) V_\mu. \end{aligned} \tag{3.18}$$

We should also note that such tensor also projects 4-dimensional tensors since $e_i^\mu n_\mu = 0$ [31] and allows to decompose the 4-metric into tangential and normal parts $g^{\mu\nu} = h^{ij} e_i^\mu e_j^\nu + n^\mu n^\nu$. With the help of the tensors in (3.6) and (3.17) we can restrict our analysis to tangent tensor fields since we can always project those that are not [30].

In $\mathcal{M}$ we have the covariant derivative ∇_μ and we wish to determine how to differentiate tangent tensor fields. A natural way would be to project the result of the covariant derivative of a tangent 4-vector V_ν, that is, we define the covariant derivative D_i of a 3-vector as:

$$\begin{aligned} D_i V_j &\equiv e_i^\mu e_j^\nu \nabla_\mu V_\nu \\ &= \nabla_\mu (V_\nu e_j^\nu) e_i^\mu - V_\nu e_i^\mu \nabla_\mu e_j^\nu \\ &= \partial_\mu V_j e_i^\mu - V_\nu e_i^\mu \nabla_\mu (g^{\nu\alpha} e_{\alpha j}) \\ &= \partial_\mu V_j \frac{\partial x^\mu}{\partial y^i} - V^\alpha e_i^\mu \nabla_\mu e_{\alpha j} \\ &= \partial_i V_j - e^{\alpha k} e_i^\mu (\nabla_\mu e_{\alpha j}) V_k. \end{aligned} \tag{3.19}$$

If we define

$$\Gamma^k_{ij} = e^{\alpha k} e_i^\mu (\nabla_\mu e_{\alpha j}), \tag{3.20}$$

we get

$$D_i V_j = \partial_i V_j - \Gamma^k_{ij} V_k. \tag{3.21}$$

It can be proven that the result of projecting the covariant derivative of the 3-metric in 4-dimensional form (equation (3.17)) is zero [30]. Hence, by unicity [22], the coefficients in equation (3.20) must be the same coefficients of the affine connection

$$\Gamma^k_{ij} = \frac{1}{2} h^{kl} \left(\partial_j h_{il} + \partial_i h_{lj} - \partial_l h_{ij} \right). \tag{3.22}$$

The last result shows that the **intrinsic covariant derivative** is the same operation as the covariant derivative in the 3-manifold Σ with the 3-metric h_{ij}. Analysing equation (3.19) it is clear that $e^\mu_i e^\nu_j \nabla_\mu A_\nu$ is the projection of the vector $e^\mu_i \nabla_\mu A^\nu$. Its normal component will give us information about how the hypersurface is embedded in the 4-dimensional space-time. In particular, we are interested in the normal component of $e^\mu_i \nabla_\mu e^\nu_j$. Using equation (3.17) we get

$$\begin{aligned} e^\mu_i \nabla_\mu e^\nu_j &= g^\nu_\rho e^\mu_i \nabla_\mu e^\rho_j \\ &= (h^{kn} e_{\rho k} e^\nu_n - n_\rho n^\nu) e^\mu_i \nabla_\mu e^\rho_j \\ &= h^{kn} e_{\rho k} e^\nu_n e^\mu_i \nabla_\mu e^\rho_j - n_\rho n^\nu e^\mu_i \nabla_\mu e^\rho_j \\ &= (e^{\rho k} e^\mu_i \nabla_\mu e_{\rho j}) e^\nu_n - (n_\rho e^\mu_i \nabla_\mu e^\rho_j) n^\nu \\ &= (\Gamma^n_{ij}) e^\nu_n - (e^\mu_i (\nabla_\mu (e^\rho_j n_\rho) - e^\rho_j \nabla_\mu (n_\rho))) n^\nu \\ &= (\Gamma^n_{ij}) e^\nu_n + (e^\mu_i e^\rho_j \nabla_\mu n_\rho) n^\nu \\ &= (\Gamma^n_{ij}) e^\nu_n + (K_{ij}) n^\nu \end{aligned} \tag{3.23}$$

where we have decomposed $e^\mu_i \nabla_\mu e^\nu_j$ in tangent and normal components and have defined the normal component as:

$$K_{ij} = e^\mu_i e^\rho_j \nabla_\mu n_\rho. \tag{3.24}$$

This quantity is the **extrinsic curvature**. In 2-dimensional surfaces it is known as the normal curvature. Although it is not clear from the definition, the extrinsic curvature is a symmetric tensor. We shall not prove that fact but a proof can be found in the references [30] or [9]. The tensors h_{ij} and K_{ij}, taken together, gather all the information about Σ. The 3-metric deals with the intrinsic characteristics and the curvature deals with the extrinsic characteristics. Above all, it should be possible to write the 4-dimensional Riemann tensor in terms of these quantities. To do that we introduce first the *Gauss* equation [5]

$$R_{\mu\nu\alpha\beta} e^\mu_i e^\nu_j e^\alpha_k e^\beta_n = R_{ijkn} + K_{ik} K_{jn} - K_{in} K_{jk}. \tag{3.25}$$

It will be useful in the following calculation. The next step is to calculate the 4-dimensional Ricci scalar directly using the 4-metric in (3.17).

$$\begin{aligned}
R &= g^{\alpha\beta}g^{\mu\nu}R_{\mu\alpha\nu\beta} \\
&= g^{\alpha\beta}(h^{ij}e_i^\mu e_j^\nu - n^\mu n^\nu)R_{\mu\alpha\nu\beta} \\
&= g^{\alpha\beta}(h^{ij}R_{\mu\alpha\nu\beta}e_i^\mu e_j^\nu - R_{\mu\alpha\nu\beta}n^\mu n^\nu) \\
&= (h^{kn}e_k^\alpha e_n^\beta - n^\alpha n^\beta)(h^{ij}R_{\mu\alpha\nu\beta}e_i^\mu e_j^\nu - R_{\mu\alpha\nu\beta}n^\mu n^\nu) \\
&= h^{kn}h^{ij}R_{\mu\alpha\nu\beta}e_i^\mu e_j^\nu e_k^\alpha e_n^\beta - h^{ij}R_{\mu\alpha\nu\beta}e_i^\mu e_j^\nu n^\alpha n^\beta \\
&\qquad - h^{kn}R_{\mu\alpha\nu\beta}n^\mu n^\nu e_k^\alpha e_n^\beta + R_{\mu\alpha\nu\beta}n^\mu n^\nu n^\alpha n^\beta \\
&= h^{kn}h^{ij}R_{\mu\alpha\nu\beta}e_i^\mu e_j^\nu e_k^\alpha e_n^\beta - 2h^{ij}R_{\mu\alpha\nu\beta}n^\mu n^\nu e_i^\alpha e_j^\beta \\
&= h^{kn}h^{ij}(R_{\mu\alpha\nu\beta}e_i^\mu e_j^\nu e_k^\alpha e_n^\beta) - 2(h^{ij}e_i^\alpha e_j^\beta)R_{\mu\alpha\nu\beta}n^\mu n^\nu \\
&= h^{kn}h^{ij}(R_{ikjn} + K_{ij}K_{kn} - K_{in}K_{kj}) - 2(g^{\alpha\beta} + n^\alpha n^\beta)R_{\mu\alpha\nu\beta}n^\mu n^\nu \\
&= ({}^{(3)}R + K^2 - K^{ij}K_{ij}) - 2R_{\mu\nu}n^\mu n^\nu, \qquad (3.26)
\end{aligned}$$

where ${}^{(3)}R$ is the 3-dimensional Ricci scalar and $K = h^{ij}K_{ij}$. To finish our calculation we need to find an expression for $R_{\mu\nu}n^\mu n^\nu$. From the definition of the Riemann tensor [9], it follows that

$$\begin{aligned}
R_{\mu\nu}n^\mu n^\nu &= (\nabla_\nu\nabla_\mu n^\mu)n^\nu - (\nabla_\mu\nabla_\nu n^\mu)n^\nu \\
&= \nabla_\nu(n^\nu\nabla_\mu n^\mu) - (\nabla_\nu n^\nu)(\nabla_\mu n^\mu) - \nabla_\mu(n^\nu\nabla_\nu n^\mu) + (\nabla_\mu n^\nu)(\nabla_\nu n^\mu) \\
&= \nabla_\nu(n^\nu\nabla_\mu n^\mu) - K^2 - \nabla_\mu(n^\nu\nabla_\nu n^\mu) + g^{\nu\alpha}g^{\mu\beta}(\nabla_\mu n_\alpha)(\nabla_\nu n_\beta) \\
&= \nabla_\nu(n^\nu\nabla_\mu n^\mu) - K^2 - \nabla_\mu(n^\nu\nabla_\nu n^\mu) + g^{\nu\alpha}g^{\mu\beta}(\nabla_\mu n_\alpha)(\nabla_\nu n_\beta) \\
&= \nabla_\nu(n^\nu\nabla_\mu n^\mu) - K^2 - \nabla_\mu(n^\nu\nabla_\nu n^\mu) + h^{ij}e_i^\nu e_j^\alpha h^{kn}e_k^\mu e_n^\beta(\nabla_\mu n_\alpha)(\nabla_\nu n_\beta) \\
&= \nabla_\nu(n^\nu\nabla_\mu n^\mu) - K^2 - \nabla_\mu(n^\nu\nabla_\nu n^\mu) + K^{ij}K_{ij} \\
&= K^{ij}K_{ij} - K^2 + \nabla_\mu\left(n^\nu\nabla_\nu n^\mu - n^\mu\nabla_\nu n^\nu\right), \qquad (3.27)
\end{aligned}$$

where we have used equation (3.17), the fact that n^ν is normalized and that the extrinsic curvature is a symmetric tensor. Putting all the results together we get

$$R = ({}^{(3)}R - K^2 + K^{ij}K_{ij}) - 2\nabla_\mu \left(n^\nu \nabla_\nu n^\mu - n^\mu \nabla_\nu n^\nu\right). \tag{3.28}$$

3.1.3 ADM Hamiltonian

Collecting the results of the last section, the action in (3.1) takes the form

$$S = S_G + S_B + S_{\text{N-G}}. \tag{3.29}$$

where

$$S_G = \frac{c^4}{16\pi G}\int N\sqrt{h}\left[\left({}^{(3)}R - K^2 + K^{ij}K_{ij}\right) - 2\Lambda\right] dx^4, \tag{3.30}$$

$$S_B = -\frac{c^4}{16\pi G}\int N\sqrt{h}\left[2\nabla_\mu \left(n^\nu \nabla_\nu n^\mu - n^\mu \nabla_\nu n^\nu\right)\right] dx^4, \tag{3.31}$$

and

$$S_{\text{N-G}} = \int \sqrt{-g}\left[\mathcal{L}_{\text{N-G}}\right] dx^4. \tag{3.32}$$

Note that we haven't change the form of $S_{\text{N-G}}$. We shall ignore it for now and we will talk about it later. We will also ignore S_B since it is a total divergence and leads to a surface term on integration and will not contribute to the equations of motion [9]. Now we are going to focus on S_G. Remember that the relevant variable in the gravitational Lagrangian is $g_{\mu\nu}$. We have separated the information contained in the 4-metric into the three functions N, N^i an h_{ij}. Then, to construct the gravitational Hamiltonian we need to find three independent conjugate momenta, one for each function. The conjugate momenta are defined in the usual manner:

$$\Pi^{ij} = \frac{\delta \mathcal{L}_{\text{ADM}}}{\delta \dot{h}_{ij}}. \tag{3.33}$$

$$\Pi^{i} = \frac{\delta \mathcal{L}_{\text{ADM}}}{\delta \dot{N}_{i}}. \tag{3.34}$$

$$\Pi^{0} = \frac{\delta \mathcal{L}_{\text{ADM}}}{\delta \dot{N}}. \tag{3.35}$$

Where

$$\mathcal{L}_{ADM} = \frac{c^4}{16\pi G} N\sqrt{h}\left[\left({}^{(3)}R - K^2 + K^{ij}K_{ij}\right) - 2\Lambda\right]. \tag{3.36}$$

It should be stressed that even though the dot " $\cdot$ " means *evolution*, it does not necessarily represents the time derivative ∂_t. It actually represents the Lie dragging along the time evolution 4-vector t^μ. In adapted coordinates, which are the ones we are using, such Lie dragging reduces to the time derivative ∂_t[33]. It is clear that we need to express the extrinsic curvature as a function of the three variables to calculate the derivatives. With equations (3.14) and (3.15) we get

$$\begin{aligned}
K_{ij} &= \nabla_i n_j \\
&= N\Gamma^0_{ij} \\
&= N\left(g^{00}\Gamma_{0ij} + g^{0k}\Gamma_{kij}\right) \\
&= N\left(-\frac{1}{2N^2}\left(\partial_j g_{0i} + \partial_i g_{0j} + \partial_0 g_{ij}\right) + \frac{1}{N^2}N^k\Gamma_{kij}\right) \\
&= N\left(-\frac{1}{2N^2}\left(\partial_j N_i + \partial_i N_j + \dot{h}_{ij}\right) + \frac{1}{N^2}N^k\Gamma_{kij}\right) \\
&= -\frac{1}{2N}\left(D_i N_j + D_j N_i - \dot{h}_{ij}\right).
\end{aligned} \tag{3.37}$$

By re-expressing the Lagrangian density

$$\mathcal{L}_{ADM} = \frac{c^4}{16\pi G} N\sqrt{h}\left[\left({}^{(3)}R + \left(h^{ik}h^{jn} - h^{ij}h^{kl}\right) K_{ij}K_{kn}\right) - 2\Lambda\right], \tag{3.38}$$

and using equation (3.37), the canonical momenta are easily calculated

$$\Pi^{ij} = \frac{c^4}{16\pi G}\sqrt{h}(K^{ij} - h^{ij}K). \tag{3.39}$$

$$\Pi^{i} = 0. \tag{3.40}$$

$$\Pi^{0} = 0. \tag{3.41}$$

From these results we recognize several facts. The Lagrangian is *singular*. Equations (3.40) and (3.41) tell us that N and N^i are not dynamical variables and should be interpreted as primary constrains (in Dirac's terminology) that will play the role of Lagrange multipliers which will be related to a gauge freedom. This should not come as a surprise since the lapse function and shift vector specify the initial foliation which is, in principle, completely arbitrary. The only dynamical variable is then h_{ij}. With equations (3.37), (3.39), (3.40) and (3.41) we can find the Hamiltonian density

$$\begin{aligned}
\mathcal{H} &= \Pi^{ij}\dot{h}_{ij} - \mathcal{L}_{\mathcal{ADM}} \\
&= \frac{c^4}{16\pi G}\sqrt{h}\left(k^{ij} - h^{ij}K\right)\left(2NK_{ij} - D_iN_j - D_jN_i\right) \\
&\quad - \frac{c^4}{16\pi G}N\sqrt{h}\left[{}^{(3)}R - K^2 + K^{ij}K_{ij} - 2\Lambda\right] \\
&= \frac{c^4}{16\pi G}\Big[N\left(K^{ij}K_{ij} - K^2 - {}^{(3)}R + 2\Lambda\right)\sqrt{h} \\
&\quad + 2N_iD_j\left(K^{ij} - h^{ij}K\right)\sqrt{h} - 2D_j\left[\left(K^{ij} - h^{ij}K\right)N_i\sqrt{h}\right]\Big].
\end{aligned} \tag{3.42}$$

Ignoring the total divergence term again, the ADM Hamiltonian becomes

$$\begin{aligned} H_{ADM} &= \frac{c^4}{16\pi G}\int_{\Sigma_t}\Big[N\left(K^{ij}K_{ij}-K^2-{}^{(3)}R+2\Lambda\right) \\ &\quad + 2N_iD_j\left(K^{ij}-h^{ij}K\right)\Big]\sqrt{h}dy^3. \end{aligned} \tag{3.43}$$

Clearly, in this Hamiltonian, the extrinsic curvature should be written a function of the conjugate momenta Π^{ij} by inverting equation (3.39)

$$K^{ij} = \frac{16\pi G}{c^4}\frac{1}{\sqrt{h}}\left(\Pi^{ij}-\frac{1}{2}h^{ij}\Pi\right). \tag{3.44}$$

If we include Π^0 and Π^i we can write the action as:

$$S = \int_{t_1}^{t_2}\int_{\Sigma_t}\left[\dot{h}_{ij}\Pi^{ij}-\Pi^0\dot{N}-\Pi^i\dot{N}_i-NH-N_iH^i\right]dy^3dt, \tag{3.45}$$

where H and H^i are obtained by comparison with (3.43)

$$H = \frac{c^4}{16\pi G}\left(K^{ij}K_{ij}-K^2-{}^{(3)}R+2\Lambda\right)\sqrt{h} \tag{3.46}$$

$$H^i = \frac{c^4}{8\pi G}D_j\left(K^{ij}-h^{ij}K\right)\sqrt{h} \tag{3.47}$$

Minimization of the action is equivalent to Hamilton's equations $\frac{\partial H}{\partial q} = -\dot{p}$ and $\frac{\partial H}{\partial p} = \dot{q}$ and with them we recover Einstein's field equation. Since the we do not want to derive Einstein's field equation, we are not going to include the calculations of the functional derivatives of the Hamiltonian with respect to Π^{ij} and h_{ij}. They can be found in [30]. Specifically, we are interested in the functional derivatives with respect to the lapse function and shift vector because they will give rise to the *secondary* constraints according to Dirac's terminology and play a central role in Dirac's quantization scheme.

$$\frac{\delta H_{ADM}}{\delta N} = -\Pi^i = H = 0. \tag{3.48}$$

$$\frac{\delta H_{ADM}}{\delta N_i} = \Pi^0 = H^i = 0. \tag{3.49}$$

Equations (3.48) and (3.49) are called the **Hamiltonian constraint** and the **Momentum constraint** respectively. The Hamiltonian constraint provides the description of the intrinsic dynamics of the gravitational field. Said classical dynamics takes place in a space called **super-space**: the space of all 3-metrics and scalar field configurations $(h_{ij}(\mathbf{y}), \Phi(\mathbf{y}))$ on a space-like hyper-surface. Equation (3.45) together with Hamilton's equations for such action are the final results of the ADM formalism. Although it seems to be against Einstein's ideas of space-time geometry, at some point we wish to obtain an equation consistent, at some level, with both quantum mechanics and general relativity. In general relativity, provided that the manifold is globally hyperbolic, the evolution of the space-time manifold given by Einstein's field equation is completely equivalent to those we have derived; and in quantum mechanics, time is an evolution parameter and not an operator [34]. With this in mind the $1+3$ split we have presented in this chapter becomes the most natural and conservative path towards a theory of quantum gravity.

3.1.4 Non-Gravitational Action

So far in our discussion we have deliberately ignored the non-gravitational field action $S_{\text{N-G}}$. Then, the Hamiltonian action of the last section would reproduce Einstein's field equation for vacuum. However, there are two ways it can be easily modified to take into account said fields. Both ways are equivalent. One way consists in using the fact that the non-gravitational Lagrangian depends on some scalar fields[1] Φ_i, its first derivatives and the 4-metric $g_{\mu\nu}$. That is $L = L\left(\Phi_i, \partial_\mu \Phi_i; g_{\mu\nu}\right)$. With this 4-metric dependence, the Lagrangian can be put through the $1+3$ splitting using equations (3.14) and (3.15). For each scalar field, a conjugate momentum is calculated in the usual way and finally the action is put in Hamiltonian form and added to the total action. It is possible to study many inflationary models by specifying the non-gravitational field with a single scalar field Φ with a potential $V(\Phi)$. The non-gravitational action will be

$$\begin{aligned}
S_{\text{N-G}} &= \int \mathcal{L}_{\text{N-G}} dx^4 \\
&= \int \Big[-\frac{1}{2} g^{\mu\nu} \partial_\nu \Phi \partial_\mu \Phi - V(\Phi) \Big] \sqrt{-g} dx^4 \\
&= \int \Big[-\frac{1}{2} \left(g^{00} \dot{\Phi}^2 + 2 g^{i0} \dot{\Phi} \partial_i \Phi + g^{ij} \partial_i \Phi \partial_j \Phi \right) - V(\Phi) \Big] N \sqrt{h} dx^4 \\
&= \int \Big[-\frac{1}{2} \Big(-N^{-2} \dot{\Phi}^2 + 2 N^{-2} N^i \dot{\Phi} \partial_i \Phi \\
&\qquad + \left(h^{ij} - N^{-2} N^i N^j \right) \partial_i \Phi \partial_j \Phi \Big) - V(\Phi) \Big] N \sqrt{h} dx^4,
\end{aligned} \tag{3.50}$$

where we used (3.15) in the last line. The conjugate momentum is

$$\Pi_\Phi = \frac{\delta \mathcal{L}_{\text{N-G}}}{\delta \Phi} = \frac{\sqrt{h}}{N} \left(\dot{\Phi} - N^i \partial_i \Phi \right). \tag{3.51}$$

The term $\Pi_\Phi \dot{\Phi} - \mathcal{L}_{\text{N-G}}$ should be added to equation (3.42) and by factoring the functions N and N_i (as we did) the constraints are automatically redefined. The other way consist on using Einstein's field equation

$$G_{\mu\nu} = R_{\mu\nu} - \frac{1}{2} g_{\mu\nu} R = \frac{8\pi G}{c^4} T_{\mu\nu}. \tag{3.52}$$

With equations (3.26) and (3.27) and a little algebra we get the equations [30]

[1]In this case the subscript i is used to count different scalar fields and not the space components of a tensor.

$$G_{\mu\nu}n^\mu n^\nu = \frac{8\pi G}{c^4}T_{\mu\nu}n^\mu n^\nu = {}^{(3)}R + K^2 - K^{ij}K_{ij} \tag{3.53}$$

and

$$G_{\mu\nu}e_i^\mu n^\nu = \frac{8\pi G}{c^4}T_{\mu\nu}e_i^\mu n^\nu = D_j\left(K^{ij} - h^{ij}K\right). \tag{3.54}$$

Since we are using adapted coordinates, with the last two equations the constraints can be rewritten as:

$$H = \frac{c^4}{16\pi G}\left(K^{ij}K_{ij} - K^2 - {}^{(3)}R + 2\Lambda + \frac{8\pi G}{c^4}T^{00}\right)\sqrt{h}, \tag{3.55}$$

and

$$H^i = \frac{c^4}{8\pi G}\left[D_j\left(K^{ij} - h^{ij}K\right) - \frac{8\pi G}{c^4}T^{i0}\right]\sqrt{h}. \tag{3.56}$$

3.2 Canonical Quantization

Having derived a Hamiltonian that describes general relativity, the next step in our road towards the Wheeler-DeWitt equation lies in Dirac's quantization programme. In short, canonical quantization consists in replacing the classical observables A, that are functions on a phase space, by self-adjoint operators $\hat{A}$ acting on some Hilbert space. This replacement is such that the commutator of two operators is given by the operator corresponding to the Poisson bracket of the observables at least up to the leading term of $\hbar$

$$\widehat{[A, B]} = i\hbar\{\hat{A}, \hat{B}\} + O(\hbar^2). \tag{3.57}$$

The term $O(\hbar^2)$ appears because the correspondence between Poisson brackets and commutators only holds *modulo factor ordering* (more on that later). We usually take the configuration variables q and momenta p as the basic observables and define a representation of them as quantum operators (that should be irreducible) as $q \to \hat{q} = q$ and $p \to \hat{p} = -i\hbar\frac{\delta}{\delta q}$. The Hamiltonian, as a function of the configuration and momenta, is promoted to the status of evolution operator giving rise to a Schrödinger equation

$$\hat{H}\left|\Psi\right\rangle = i\hbar\frac{d}{dt}\left|\Psi\right\rangle, \tag{3.58}$$

where $\left|\Psi\right\rangle$ is a state vector of the appropriate Hilbert space. This procedure is valid for regular systems. For singular system (a system with constraints) we do not get a Schrödinger equation like (3.58) but a series of conditions (one for each constraint) to be imposed on the state vector $\left|\Psi\right\rangle$ of the form $\hat{H}\left|\Psi\right\rangle = 0$. We devote appendix A to a more complete summary of the quantization of constrained systems. In the case of general relativity we have the variables h_{ij}, N, N_i, Φ which are going to turn into operators $\hat{h}_{ij}$, $\hat{N}$, $\hat{N}_i$, $\hat{\Phi}$. The momentum operators related to each variable are

$$\hat{\Pi}^{ij} = -i\hbar\frac{\delta}{\delta h_{ij}}, \quad \hat{\Pi}^{0} = -i\hbar\frac{\delta}{\delta N}, \quad \hat{\Pi}^{i} = -i\hbar\frac{\delta}{\delta N_i}, \quad \hat{\Pi}_{\Phi} = -i\hbar\frac{\delta}{\delta \Phi}. \tag{3.59}$$

Using the **DeWitt metric** $G_{ijkl} = \frac{1}{2\sqrt{h}}\left(h_{ik}h_{jl} + h_{il}h_{jk} - h_{ij}h_{kl}\right)$, it is possible to rewrite the Hamiltonian constraint (3.55) as

$$H = \frac{16\pi G}{c^4}G_{ijkl}\Pi^{ij}\Pi^{kl} - \frac{c^4}{16\pi G}\sqrt{h}\left({}^{(3)}R - 2\Lambda\right) + T^{00}\left(\Phi, \Pi_{\Phi}\right) = 0. \tag{3.60}$$

Here $T^{00}\left(\Phi, \Pi_{\Phi}\right) = -\frac{1}{2h}\Pi_{\Phi}^2 + \frac{1}{2}h^{ij}\partial_i\Phi\partial_j\Phi + V(\Phi)$. After quantization, that is, after substituting the operators in equation (3.59) and ignoring the factor ordering issues, the Hamiltonian constraint becomes

$$\left[\frac{16\pi G\hbar^2}{c^4}G_{ijkl}\frac{\delta}{\delta h_{ij}}\frac{\delta}{\delta h_{kl}} + \frac{c^4}{16\pi G}\sqrt{h}\left({}^{(3)}R - 2\Lambda\right) - \hat{T}^{00}\left(\Phi, \hat{\Pi}_{\Phi}\right)\right]\Psi\left[h, \Phi\right] = 0. \tag{3.61}$$

This is the **General Wheeler-DeWitt equation** $\hat{H}\Psi\left[h_{ij},\Phi\right]=0$. In this equation the quantum state of the system is represented by a wave functional $\Psi\left[h_{ij},\Phi\right]$ on the super-space. It important to note that, unlike ordinary quantum mechanics, this equation does not depend explicitly on some evolution parameter t. The reason being that the Einstein-Hilbert action is time re-parametrization invariant and the time parameter is already contained within the 3-metric and the scalar field [35]. This fact has caused much confusion and there are several ways to interpret this fact which we will mention next chapter. The Wheeler-DeWitt equation is a second order hyperbolic functional differential equation on super-space. Due to factor ordering such equation is not well-defined although there are different choices that can be made for different calculations [2]. We will address this issue later too. The other three constraints are the conditions

$$\begin{aligned} -i\hbar\frac{\delta\Psi\left[h_{ij},\Phi\right]}{\delta N} &= 0 \\ -i\hbar\frac{\delta\Psi\left[h_{ij},\Phi\right]}{\delta N_i} &= 0, \end{aligned} \tag{3.62}$$

and

$$\left[-i\hbar D_j\Pi^{ij}+\hat{T}^{i0}\right]\Psi\left[h_{ij},\Phi\right]=0, \tag{3.63}$$

where $\hat{T}^{i0}=h^{ij}\partial_j\Pi_\Psi$. Conditions (3.62) imply that the wave function does not depend on the lapse function and the shift vector. Again, this is fact should be expected due to the nature of these variables. The momentum constraint (3.63) implies that the wave functions remain unchanged for configurations $(h_{ij}(\mathbf{y}),\Phi(\mathbf{y}))$ in the super-space related by a coordinate transformation in the hyper-surface [35] (diffeomorphism invariance).

The wheeler-DeWitt equation is the cornerstone of canonical quantum gravity. Although it is the result of applying traditional, simple and direct methods (a good path to follow trying to obtain a theory of which we have little to no insight), making it a rather conservative approach, the wheeler-DeWitt has been highly criticized since its appearance. In the next chapter we will review some of the problems that have been the source of the criticism.

Chapter 4

Applications, Issues and Predictions of the Wheeler-DeWitt Equation

Lets start this chapter with two quotes by Christopher Isham: "...In the most popular approach, the constraints are imposed on the state vectors and give rise to the famous Wheeler-DeWitt equation arguably one of the most elegant equations in theoretical physics, and certainly one of the most mathematically ill-defined" [36]. "...although it may be heretical to suggest it, the Wheeler-DeWitt equation -elegant though it be- may be completely the wrong way of formulating a quantum theory of gravity" [37].

The canonical procedure discussed in the last chapter is the most criticized approach to a theory of quantum gravity. As we shall see, the criticism arises from conceptual and technical problems surrounding the Wheeler-DeWitt equation and its derivation. In this section we will discuss the most important issues in the context of quantum cosmology.

4.1 Example: The FRW Model

Since the super-space is infinite dimensional, solving the Wheeler-DeWitt equation is virtually impossible so, to be able to analyse the dynamics of the Wheeler-DeWitt and draw useful conclusions, an infinite number of degrees of freedom must be fixed [2]. This means using the equation for a determined model of the universe. In this section, our objective is to obtain the Wheeler-DeWitt equation for in the special case of an homogeneous isotropic model. The starting point for deriving the Wheeler-DeWitt equation for a concrete model is the Einstein-Hilbert action (equation (3.1)), where R is the Ricci scalar, Λ denotes the cosmological constant, g represents the determinant of the metric, κ is the curvature and integration is carried out over all space-time. For simplicity we will set $k^2 = \frac{8\pi G}{c^4}$, so that the action reads

$$S = \int \sqrt{-g} \frac{1}{2k^2} \left[R - 2\Lambda \right] dx^4 + S_{\text{N-G}}. \tag{4.1}$$

We want to apply the formalism for the case of a Friedmann universe, which is, as discussed earlier, of central relevance for quantum cosmology. In the homogeneous and isotropic universe the line element is given by equation (2.8) in chapter 2. Note that, comparing with equation (3.13), in such metric the factor N is set to one. This means that the foliation has been already chosen in the conventional Friedmann time, given by a comoving observer. The cosmological fluid will be represented by a single scalar field Φ with a potential $V(\Phi)$ (enough for many inflationary models). Using equations (3.13) and (2.12) we can write the action as

$$S = \frac{6\pi^2}{k^2} \int \left(-a\dot{a}^2 + \kappa a - \frac{\Lambda a^3}{3} \right) dt + \pi^2 \int a^3 \left(\dot{\Phi} - 2V(\Phi) \right) dt. \tag{4.2}$$

Where we have integrated out the angular degrees of freedom giving $2\pi^2$ (the volume of a spatial hyper-surface). We thus have a Lagrangian of a system with two degrees of freedom, namely: the scale factor a, and the scalar field Φ. To continue with our quantization we must calculate the conjugate momenta for each variable.

$$\Pi_a = \frac{\partial \mathcal{L}}{\partial \dot{a}} = -\frac{6a\dot{a}}{k^2} \quad , \qquad \Pi_\Phi = \frac{\partial \mathcal{L}}{\partial \dot{\Phi}} = a^3\dot{\Phi}. \tag{4.3}$$

Inverting these relations we can find the Hamiltonian

$$\begin{aligned} \mathcal{H} &= \Pi_a \dot{a} + \Pi_\Phi \dot{\Phi} - \mathcal{L} \\ &= -\frac{k^2}{12a}{\Pi_a}^2 + \frac{1}{2a^3}{\Pi_\Phi}^2 + \frac{\Lambda a^3}{k^2} - \frac{3\kappa a}{k^2} + a^3 V(\Phi). \end{aligned} \tag{4.4}$$

Since we are considering a homogeneous isotropic universe, equation (3.63), the momentum constraint, is satisfied trivially (see discussion on page 40). Comparing the Hamiltonian density with equation (3.60) we can find the DeWitt metric by inspection.

$$G_{ij} = \begin{pmatrix} -\frac{6a}{k^2} & 0 \\ 0 & a^3 \end{pmatrix}. \tag{4.5}$$

Our mini-super-space, the space spanned by the canonical variables (a, Φ), has dimension 2, hence the DeWitt metric has such form. The Hamiltonian constraint requires us to set equation (4.21) to zero and applying Dirac's canonical quantization and ignoring factor ordering issues we get

$$\left(\frac{\hbar^2 k^2}{12a}\frac{\partial^2}{\partial a^2} - \frac{\hbar^2}{2}\frac{\partial^2}{\partial \Phi^2} + a^6 \left(V(\Phi) + \frac{\Lambda}{k^2} \right) - \frac{3\kappa a^3}{k^2} \right) \Psi\left[a, \Phi\right] = 0. \tag{4.6}$$

The methods described in this chapter provide us with an equation with form of the Klein-Gordon equation in quantum field theory. The derivative with respect to the scale factor corresponds to a time derivative and the derivative with respect to the scalar field corresponds to a space derivative [38]. This equation plays the central role in quantum cosmology in the same sense that the Schrödinger equation plays a central role in quantum mechanics. Of course there are differences between equation (4.6) and the Schrödinger equation and we will discuss them in the next chapter.

4.1.1 Tunnelling and Inflation

As we discussed in the last chapter, inflation tries to solve various problems in classical cosmology. However, there is no motivation for inflation other than the solving these problems and if inflation is to be a realistic solution then it should predicted by a theory of quantum cosmology. In the quantized FRW model a connection between tunnelling and inflation can be made (see [6] and the references therein). Lets consider an empty universe with cosmological constant Λ. In this case there is no scalar field and the Wheeler-DeWitt equation becomes

$$\left(\frac{\hbar^2 k^2}{12a}\frac{\partial^2}{\partial a^2} + \frac{\Lambda a^3}{k^2} - \frac{3\kappa a}{k^2}\right)\Psi\left[a\right] = 0. \tag{4.7}$$

This equation has the same form of a one dimensional Schrödinger equation for a particle moving in a potential

$$U(a) = \frac{36}{k^4}\left(\kappa a^2 - \frac{\Lambda a^4}{3}\right), \tag{4.8}$$

constrained to have zero total energy. In particular, for a closed universe ($\kappa = +1$), in the analogy of a moving particle, this potential has a very special shape. As shown in figure 4.1, $U(a)$ presents a classically forbidden region for values $0 \leq a \leq a_0$. However, we know that quantum mechanically there is a non-zero probability that the particle can tunnel through the potential and appear in the classically allowed region for values $a \geq a_0$. So, it is possible for a closed empty universe to be created by means of a tunnelling phenomenon.

The connection can be made more explicit as follows. Having equation (2.23)

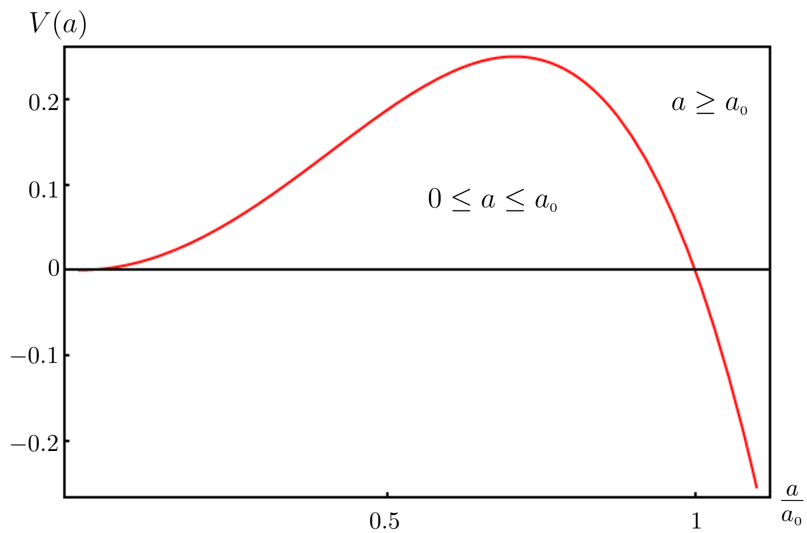

Figure 4.1: Potential $U(a)$ of the Wheeler-DeWitt equation for the FRW model.

in mind, if the universe is dominated by a term of the form A/a^n with constant A, then the scale factor behaves as

$$a(t) = t^{\frac{2}{n}}. \tag{4.9}$$

For radiation $n = 4$ and for matter $n = 3$. In the case of a decaying cosmological constant we have

$$\Lambda = \frac{A}{a^n}. \tag{4.10}$$

Inflation implies a positive acceleration. Using this in equation (4.9) we find that n must be smaller than 2. Inserting equation (4.10) in the potential (4.8) we get the condition

$$U(a) = \frac{36}{k^4}\left(a^2 - \frac{Aa^{4-n}}{3}\right). \tag{4.11}$$

A decaying cosmological constant cannot be considered in an empty universe

[6] and we need to add a non-zero density term, but by inspecting equation (4.6) for closed universes we see that the potential is the same as (4.11) with a constant term B.

$$U(a) = \frac{36}{k^4}\left(a^2 - \frac{Aa^{4-n}}{3} - B\right). \tag{4.12}$$

Clearly this potential will give tunnelling solutions if and only if $n < 2$. Thus the condition for quantum tunnelling solutions is equivalent to the condition for classical inflation. The argument can be generalized even further by considering a non-zero scalar field. The density and pressure for an interacting scalar field Ψ are $\rho = \dot{\Phi}^2/2 + V(\Phi)$ and $p = \dot{\Phi}^2/2 - V(\Phi)$. Using equation (2.18) and ignoring the cosmological constant we find

$$\frac{\ddot{a}}{a} = -\frac{k^2}{3}\left(\dot{\Phi}^2 - V(\Psi)\right). \tag{4.13}$$

Inflation is only possible if $\dot{\Phi}^2 < V(\Phi)$. In the slow roll approximation we assume that the field is constant and the inflation conditions becomes $0 < V(\Phi)$. On the other hand, using equation (4.6) we find a potential

$$U(a) = \frac{36}{k^4}\left(a^2 - \frac{k^2 V(\Phi)a^4}{3}\right). \tag{4.14}$$

In this case the potential depends on both the scalar field and the scale factor, so tunneling can occur in either direction. Though, as in equation (4.13), this potential allows tunnelling solutions in the a direction if $0 < V(\Phi)$, which is the same condition for inflation in the classical case emphasizing the relation between inflation and quantum tunnelling.

4.2 The Problem of Time

The concepts of time in general relativity and classical mechanics very different. Then, it shouldn't come as a surprise that this mismatch of concepts would cause problems when trying to find a quantum theory of gravitation via canonical quantization. In quantum mechanics, time is measured by an external clock, meaning that it is not part of the system we are trying to describe. On the other hand, time is dynamical in general relativity. As we have mention before and what is obvious examining equation (3.61), the Wheeler-DeWitt equation is defined in the configuration space and lacks a first derivative in time with an imaginary factor. This is known as the problem of time. It should be noted that all we have done so far has been done for quantum field theory, yet in such a theory there is no problem of time like in quantum gravity. The reason is that the external time in quantum mechanics is replaced by another *external* parameter in quantum field theory: the Minkowski metric $\eta_{\mu\nu}$. Since it is constant, the Minkowski space-time plays the role of external time. Principally following [37], we shall discuss the three categories of possible solutions to this problem.

4.2.1 Time Before Quantization

The main idea here is to find a functional of the canonical variables that will play the role of an external time before using Dirac's canonical quantization such that a Schrödinger-like equation is obtained. In this approach is based in eliminating the non-dynamical degrees of freedom. In phase space the gravitational waves have four dynamical degrees of freedom, namely, the two circular polarizations and their conjugate variables but in the theory described by the Wheeler-DeWitt equation we have a total of sixteen variables: the lapse function N, called the shift vector N^i, the components of the 3-metric and their conjugate momenta. To eliminate them we fix the lapse function and the shift vector since they are gauge variables, then we perform a canonical transformation

$$(h_{ij}(\mathbf{y}), \Pi^{ij}(\mathbf{y})) \longrightarrow (\chi^A(\mathbf{y}), P_A(\mathbf{y}); \varepsilon_r(\mathbf{y}), p^r(\mathbf{y})), \tag{4.15}$$

where χ^A $(A, B = 0, 1, 2, 3)$ specifying a particular choice coordinates and P_A

are their canonical momenta respectively. They describe how the hyper-surfaces, Σ, are embedded in the pseudo-Riemannian space-time. ε^s and p_s $(r, s = 1, 2)$ represent the two *true* degrees of freedom of the gravitational field. At this point we have only twelve degrees of freedom. We now express the action as a function o the new variables

$$S = \int_{t_1}^{t_2} \int_{\Sigma_t} \left[\chi^A P_A + \varepsilon^s p_s - NH - N_i H^i \right] dy^3 dt, \tag{4.16}$$

and solve the Hamiltonian constraint and the Momentum constraint for the variables P_A in the form

$$P_A(\mathbf{y}) + h^A(\mathbf{y}; \chi^B, \varepsilon^s, p_s) = 0 \tag{4.17}$$

to eliminate four more. Here h^A are simply remaining terms. We can remove the remaining four by replacing (4.17) into (4.16) and applying the constraints, leaving us with the expression

$$S = \int_{t_1}^{t_2} \int_{\Sigma_t} \left[\varepsilon^s p_s - h^A(\mathbf{y}; \chi^B, \varepsilon^s, p_s) \dot{\chi}^A \right] dy^3 dt. \tag{4.18}$$

We can see that equation (4.18)s describes an ordinary system using only the *true* degrees of freedom. Upon quantization we get

$$i\hbar \frac{\delta \psi \left[\varepsilon^s(\mathbf{y}) \right]}{\delta \chi^A} = h^A(\mathbf{y}; \chi^B, \varepsilon^s, p_s) \psi \left[\phi^r(\mathbf{y}) \right], \tag{4.19}$$

which is a Schrödinger-like for the state vector ψ_{χ^A}. In this scheme the theory can be equipped with a Hilbert space structure since (ε^s, p_s) are true degrees of freedom and according with quantum mechanics we should require the respective operators to be self-adjoint. This was not possible before since it is not clear if constraint operators should be self-adjoint or not. In turn, having a Hilbert space structure allows us to have probabilistic interpretations of the wave function of the universe. We can say that the probability of the universe having the field configurations corresponding to a subset C of the configuration space is [37]

$$\text{Prob}(\psi; \varepsilon \in C) = \int_C (\psi\left[\varepsilon^s(\mathbf{y}), \chi\right])^2 d\mu(\varepsilon). \tag{4.20}$$

The inner product also allows us to construct a notion of quantum observable. That is, a functional of the fields and the functions χ which are self-adjoint. In this programme, the usual rules of quantum mechanics apply and we can ask for probability distribution of the spectrum of different operators. However, there are two main problem with this approach. The first one is that there are no global solutions to the constrains for the variables P_A in general relativity. This problem can be avoided by using what is called *matter clocks* [37] [39]. By adding to the gravitational action a non-gravitational part that is linear in the momentum, global solutions to the constraints can be found, but it is clear that such matter field wouldn't describe physical matter.

The second problem is that the choice of the functions χ is not unique and the theory does not give us a hint of which one of all the possible function we should choose. We can see the severity of this problem with an example. For the FRW model the Hamiltonian is

$$\begin{aligned} \mathcal{H} &= \Pi_a \dot{a} + \Pi_\Phi \dot{\Phi} - \mathcal{L} \\ &= -\frac{k^2}{12a}{\Pi_a}^2 + \frac{1}{2a^3}{\Pi_\Phi}^2 + \frac{\Lambda a^3}{k^2} - \frac{3\kappa a}{k^2} + a^3 V(\Phi). \end{aligned} \tag{4.21}$$

A natural extrinsic time for this model and for a positive curvature ($\kappa = 1$) is the scale factor $t = a$. Following the procedure described above we need to solve the equation $\mathcal{H} = 0$ for Π_a. Doing so we get

$$\Pi_a = \pm\sqrt{+\frac{6}{k^2 t^2}{\Pi_\Phi}^2 + \frac{12\Lambda t^4}{k^4} - \frac{36 t^2}{k^4} + \frac{12 t^4 V(\Phi)}{k^2}}. \tag{4.22}$$

On the other hand we could consider using the field $t = \Phi$ as an external time.

In this case we get

$$\Pi_\Phi = \pm\sqrt{\frac{a^2k^2}{6}{\Pi_a}^2 - \frac{2\Lambda a^6}{k^2} + \frac{6a^4}{k^2} - 2a^6V(t)}. \tag{4.23}$$

These operators would give two very different Schrödinger equations and therefore would give two inequivalent predictions. Before moving on to other approaches we should mention that since the Wheeler-DeWitt equation is obtained using Dirac's programme on the action (3.45), that is, woithout solving the constraints, the equation that we get in the *time before quantization* approach is not the Wheeler-DeWitt equation. It is in fact called the *Tomonaga-Schwinger equation*, although it should have the same interpretation.

4.2.2 Time After Quantization

A different way to solve the problem of time is to find an evolution after using Dirac's quantization. As we seen, the result is the Wheeler-DeWitt equation, so the main idea is to find a Schrödinger-like equation using such equation as a starting point. This approach relies heavily on WKB methods.

So, we start with the equation

$$\left[\frac{16\pi G\hbar^2}{c^4}G_{ijkl}\frac{\delta}{\delta h_{ij}}\frac{\delta}{\delta h_{kl}} + \frac{c^4}{16\pi G}\sqrt{h}\left({}^{(3)}R - 2\Lambda\right) - \hat{T}^{00}\left(\Phi, \hat{\Pi}_\Phi\right)\right]\Psi\left[h, \Phi\right] = 0. \tag{4.24}$$

The next step is to look for solutions of the form

$$\Psi\left[h, \Phi\right] = A\left[h\right]\varphi\left[h, \Phi\right]e^{iS[h]/\hbar k^2}, \tag{4.25}$$

Where $k^2 = \frac{16\pi G}{c^4}$. We now expand φ as power series of the constant G so that

$$\varphi\left[h, \Phi\right] = \sum_{n=0}^{\infty} G^n\psi_n\left[h, \Phi\right]. \tag{4.26}$$

If we put equation (4.26) into (4.25) and then insert the result into the Wheeler-DeWitt equation we get

$$-2i\hbar G_{ijkl}\frac{\delta S\left[h\right]}{\delta h_{ij}}\frac{\delta\psi\left[h,\Phi\right]}{\delta h_{kl}}+\hat{T}^{00}\left(\Phi,\hat{\Pi}_{\Phi}\right)\psi\left[h,\Phi\right]=0. \tag{4.27}$$

The main step is to find functions $\mathbb{T}(y,h)$ and $\sigma^{r}(y,h)$, $r=1,\ldots,5$ such that the following relations hold

$$2\hbar G_{ijkl}\frac{\delta S\left[h\right]}{\delta h_{ij}}\frac{\delta\mathbb{T}(y')\left[h,\Phi\right]}{\delta h_{kl}}=\delta(y,y'). \tag{4.28}$$

$$2\hbar G_{ijkl}\frac{\delta S\left[h\right]}{\delta h_{ij}}\frac{\delta\sigma T(y')\left[h,\Phi\right]}{\delta h_{kl}}=0. \tag{4.29}$$

Once the function are found we can use them to define coordinates $(\mathbb{T},\sigma)$ in the space of Riemannian metrics (super-space). Using this coordinates we can rewrite equation (4.27) as

$$i\hbar G_{ijkl}\frac{\delta\psi\left[\mathbb{T},\sigma,h,\Phi\right]}{\delta\mathbb{T}(y)}=\hat{T}^{00}\left[\mathbb{T},\sigma,h\right]\psi\left[\mathbb{T},\sigma,h,\Phi\right]=0, \tag{4.30}$$

Which is the desired Schrödinger-like equation. In this approach only the gravitational field is treated in this semi-classical way since the phase factor S only depends on h. The matter fields are fully quantized. Equation (4.30) permits a probabilistic interpretation of the wave function but the probability associated with it is conserved only to the same order in the expansion to which is valid. This approximation, of course, breaks down at the turning points of S. Another problem is that the first-order form of the Schrödinger equation (4.30) is lost at the next order in the WKB approximation, so the traditional interpretation of quantum mechanics breaks down too as one approaches the plank scale. Since this *time* evolution is only possible at a semi-classical level, the notion of probability is also only in some approximate sense. So this programme does not solve the problem of time but it changes it for the question how to interpolate between the Schrödinger equation (4.30) and the Wheeler-DeWitt equation. It should be noted also that The WKB ansatz is only one of a very large number of possible classes of solution to the Wheeler-DeWitt equation. Even worse, it doesn't consider a superposition of WKB solutions. It is in principle possible to consider the ansatz

$$\Psi\left[h,\Phi\right]=\sum_{n}A_{n}\left[h\right]\varphi_{n}\left[h,\Phi\right]e^{iS_{n}[h]/\hbar k^{2}}, \tag{4.31}$$

but, according to the procedure discussed above, each phase factor would lead to a different definition of time. A particular example is the Hartle-Hawking proposal $e^{iS[h]/\hbar k^2}+e^{-iS[h]/\hbar k^2}$ which corresponds to expanding and contracting universes respectively [2].

4.2.3 Timeless Option

The main idea behind the *timeless* interpretations of the theory is the belief (based on some ideas of quantum mechanics) that it could be possible to have a well-defined quantum mechanical formalism without the need to use an a priori time evolution. *Timeless approach* is a misleading name since it does employ some sort of variable to keep time but such a notion of time is interpreted as purely phenomenological and devoid conceptual significance. First we the impose an inner product on the super-space

$$\langle\Psi\,|\,\Xi\rangle=\int\Psi^{*}\left[h,\phi\right]\Xi\left[h,\phi\right]D(h,\phi). \tag{4.32}$$

Where $D(h,\phi)$ is some measure defined in the super-space[1]. The use of this scalar product seems natural since $L^2(\text{super-space}, D(h,\phi))$ is the Hilbert space on which the canonical operators defined during quantization are self-adjoint. The scalar product defines a large set of square-integrable functions, many of them are non-physical but the momentum constraint and the momentum con-

[1] There are some serious difficulties around defining such measure [40] but we are not going to focus on the mathematical aspects.

straint *rule out* these states. The interpretation of $|\Psi[h,\phi]|$ however is a little delicate. It is no longer the probability of finding a hyper-surface in space-time on which the three-metric h and the field ϕ lies in the measurable subset C like in equation (4.20). Instead, by fixing any of the degrees of freedom, it represents the probability the conditional probability of finding the unfixed degrees of freedom given that the degrees of freedom remaining are fixed. The claim is that it is not necessary to split the degrees of freedom between physical and non-physical. The interpretation is supposed to be correct for any such choice. For example, in the FRW model wave function $\psi(a,\phi)$ can be regarded as the probability density in a at fixed ϕ or as the probability density in ϕ at fixed a. To understand this lets discuss first the notion of conditional probabilities in quantum mechanics. If the state of a system at a time $t=0$ is given by ρ_0, it is related to the state at a time t by the evolution operator

$$\rho_t = U\rho_0 U^{-1}. \tag{4.33}$$

If a measurement of an observable $\hat{A}$ is made at time t, the probability that the result will lie in some subset α of the spectrum of the operator is

$$\mathrm{Prob}(A\in\alpha, t; \rho_0) = \mathrm{tr}\left(P^A_\alpha \rho_t\right) = \mathrm{tr}\left(P^A_\alpha(t)\rho_0\right), \tag{4.34}$$

where P^A_α is the projection operator for the subspace α and $P^A_\alpha(t) = U^{-1}P^A_\alpha U$. If the measurement of yields a result lying in α, any further measurements must be made using the new density matrix

$$\rho_\alpha = \frac{P^A_\alpha(t)\rho_0 P^A_\alpha(t)}{\mathrm{tr}\left(P^A_\alpha(t)\rho_0\right)}. \tag{4.35}$$

So, if we make a measurement of an observable $\hat{B}$ at a time $t_1 \geq t$, the probability of obtaining a result in some subset β is

$$\mathrm{Prob}(B\in\beta, t_1|A\in\alpha, t; \rho_0) = \frac{\mathrm{tr}\left(P^B_\beta(t_1)P^A_\alpha(t)\rho_0 P^A_\alpha(t)\right)}{\mathrm{tr}\left(P^A_\alpha(t)\rho_0\right)}. \tag{4.36}$$

These ideas can be extended to quantum gravity. Due to the Hamiltonian constraint we have the expression $[H, \rho] = 0$. Hence, equation (4.36) loses the time dependence

$$\mathrm{Prob}(B \in \beta | A \in \alpha; \rho_0) = \frac{\mathrm{tr}\left(P^B_\beta P^A_\alpha \rho_0 P^A_\alpha\right)}{\mathrm{tr}\left(P^A_\alpha \rho_0\right)}. \tag{4.37}$$

Now, the only meaningful concept is the conditional probability of finding $\hat{B}$ in the range β, given that $\hat{A}$ lies in α and the system is in the state ρ_0. Since there are no time labels in (4.37) there is no reason to consider a time order for the quantities $\hat{A}$ and $\hat{B}$. As a consequence we obtain a timeless picture of quantum theory, although it is possible to study the evolution of quantities. Clearly, if T is a degree of freedom that we wish to use as a time parameter to study the change of another quantity $\hat{A}$ we simply study how $\mathrm{Prob}(A \in \alpha | T = \tau, \rho_0)$ changes with τ.

The timeless approach is certainly an elegant one but it is by no means free of problems. The main difficulty is that the probabilistic rule expressed in equation (4.37) constitutes a separation from the conventional interpretation of quantum mechanics. It is possible for the theory to not be self-consistent. Another difficulty of the conditional probability interpretation arises from the absence of any sense of history. Since there is no time there is no way of comparing things at different times in the classical view. This in turn makes it difficult to understand how the early universe and the current universe are connected.

4.2.3.1 A Few Words on the Many-Worlds

The timeless approach has some consequences on what would be a definite interpretation of a quantum theory. To see this lets us review the Copenhagen interpretation. Lets consider a quantum system S interacting with an apparatus $\mathbb{A}$ which measures the observable A of the system. Let $|\psi^s\rangle$ and $\left|\psi^A[\ldots]\right\rangle$ be the initial states of the system and the apparatus respectively. The total Hilbert space is the product of the system's Hilbert space and the apparatus' Hilbert space. First, we consider the particular case where the initial state of the system is $\hat{A}\left|\psi_m^s\right\rangle = A_m\left|\psi_m^s\right\rangle$, that is, an eigenstate of the measured operator $\hat{A}$. According with the rules of quantum mechanics, the state of the system after the interaction is the same as the initial state and the final state of the apparatus is $\left|\psi^A\left[A_m\right]\right\rangle$. In this case the evolution of the system and the apparatus can be described by means of the Schrödinger equation, menaing that there is an unitary operator U_A, such that

$$U_A(\left|\psi_m^s\right\rangle\left|\psi^A\left[\ldots\right]\right\rangle) = \left|\psi_m^s\right\rangle\left|\psi^A\left[A_m\right]\right\rangle. \tag{4.38}$$

If we now pass to the general case where the initial state of the system is an arbitrary superposition of the eigenvalues of $\hat{A}$, i.e. $\left|\psi^s\right\rangle = \sum_m A_m\left|\psi_m^s\right\rangle$, we will find a problem. From the linearity of the Schrödinger equation, the evolution of the total system is

$$U_A(\sum_m A_m\left|\psi_m^s\right\rangle\left|\psi^A\left[\ldots\right]\right\rangle) = \sum_m A_m\left|\psi_m^s\right\rangle\left|\psi^A\left[A_m\right]\right\rangle. \tag{4.39}$$

Clearly, the superposition (4.39) cannot be the result of a single measurement since it includes terms corresponding to all possible results. The question of how to interpret this equation originates different interpretations to the theory. In the Copenhagen interpretation this question is answered by invoking a *external classical observer* who is not described by the Schrödinger equation. The interaction with the external observer further collapses or reduces the total state as follows [41]

$$\text{Observer} + \sum_m A_m\left|\psi_m^s\right\rangle\left|\psi^A\left[A_m\right]\right\rangle = \left|\psi_n^s\right\rangle\left|\psi^A\left[A_n\right]\right\rangle, \tag{4.40}$$

with a priori introduced probabilities $p_n = |A_n|^2$ for some n within the size of the spectrum of $\hat{A}$. So, in such interpretation there are two inequivalent evolutions and what is worse, one of the uses a concept external to the system. On the other hand, in the many-worlds interpretation we assume that the superposition (4.39) describes the result of an ensemble of measurements and the state $|\psi^s\rangle = \sum_m A_m |\psi^s_m\rangle$ is put into correspondence with an ensemble of systems. If we assume that there are many universes and that the superposition (4.39) describes simultaneously the results of measurements made in different universes, and to each universe and each measurement corresponds one of the terms in the superposition. Then, the state $|\psi^s\rangle = \sum_m A_m |\psi^s_m\rangle$ represents an ensemble of systems but each system lives in its own universe and in any universe the quantum theory describes an individual system which is affected by corresponding system in other universes. The assumption of the existence of many universes is the core of the many-worlds interpretation. It eliminates the need of an external observer that collapses the wave function and leaves only the Schrödinger evolution. This is why Everett's interpretation is particularly attractive in a theory of quantum gravity. If we are talking about a state that describes the whole universe, it makes no sense to invoke an external observer, since by definition there is nothing outside the universe. Furthermore, this interpretation has an special affinity with the timeless approach since equation (4.37) is not obtained via any process of state collapse or reduction. Time and measurements become secondary concepts. They are not something that comes from *outside* but they are instead identified with correlations within the system, i.e. it is a way of referring to particular interactions between sub-systems of a closed system.

4.3 Operator Ordering

The problem of factor ordering is not exclusive to quantum gravity. It is an issue that comes with the procedure of quantization reviewed in the appendix A and it refers to the ambiguities in the order of which non-commuting operators should be used in a resulting equation. Although the factor ordering is very difficult to solve in quantum gravity[1], it is easy to understand its origin [42]. In writing the quantum mechanical version of a classical theory, by the correspondence principle,

[1] There are few to none rules to determine which order is the *correct* order.

it is necessary that we obtain the classical theory in the limiting process $\hbar \to 0$. This problem does not have a unique solution since, in its simplest form, there are several (and inequivalent) quantum operators $\hat{F}(\hat{q}, \hat{p})$ that approaches the classical function $F(q,p)$ in the limit $\hbar \to 0$ since commutativity is not an issue classically[1]. The Wheeler-DeWitt equation is

$$\left[\frac{16\pi G\hbar^2}{c^4} G_{ijkl} \frac{\delta}{\delta h_{ij}} \frac{\delta}{\delta h_{kl}} + \frac{c^4}{16\pi G}\sqrt{h}\left({}^{(3)}R - 2\Lambda\right) - \hat{T}^{00}\left(\Phi, \hat{\Pi}_\Phi\right)\right] \Psi\left[h, \Phi\right] = 0. \tag{4.41}$$

As shown before, the DeWitt metric is a function of the 3-metric. Hence, after promoting the coordinates of the phase space to operators, the first would involve the product of the non-commuting operators $\hat{\Pi}_{ij}$, $\hat{h}^{ij}$. In the case of quantum cosmology, in particular, for homogeneous isotropic models the classical Hamiltonian is

$$\mathcal{H} = -\frac{k^2}{12a}{\Pi_a}^2 + \frac{1}{2a^3}{\Pi_\Phi}^2 + \frac{\Lambda a^3}{k^2} - \frac{3\kappa a}{k^2} + a^3 V(\Phi). \tag{4.42}$$

The problematic term is $\frac{k^2}{12a}{\Pi_a}^2$. Examples of possible ordering are

$$\hat{\Pi}_a \hat{a}^{-1} \hat{\Pi}_a, \quad \hat{a}\hat{\Pi}_a \hat{a}^{-2} \hat{\Pi}_a, \quad \hat{a}\hat{\Pi}_a \hat{a}\hat{\Pi}_a \hat{a}^{-3}, \quad \hat{a}^2 \hat{\Pi}_a \hat{a}^{-1} \hat{\Pi}_a \hat{a}^{-2}. \tag{4.43}$$

These examples are enough motivation to use a parametrization for the ordering problem

$$\left(\frac{\hbar^2 k^2}{12} a^i \frac{\partial}{\partial a} a^j \frac{\partial}{\partial a} a^k - \frac{\hbar^2}{2}\frac{\partial^2}{\partial \Phi^2} + a^6\left(V(\Phi) + \frac{\Lambda}{k^2}\right) - \frac{3\kappa a^3}{k^2}\right)\Psi\left[a, \Phi\right] = 0. \tag{4.44}$$

where the (possibly complex) parameters i, j, k fulfil the condition $i + j + k = -1$. There are popular orderings which cosmologist have used to make calcula-

[1]Here q, p are the classical coordinates and momenta, and $\hat{q}, \hat{p}$ are their quantum counterparts. F could be, for example, a Hamiltonian.

tions. There is, for example, $j = k = 0$, $j = 1$ used by Vilenkin [43, 44, 45]. There is the pseudo-general Hartle-Hawking factor ordering $k = 0$, $j = -r$ and $i = -1 + r$ [46, 47]. And there are operator orderings that try to interpret the problematic term as a Laplace-Beltrami operator on phase space, i.e. $i = -1/4$, $j = -1/2$, $k = -1/4$ [3] and $i = -2$, $j = 1$, $k = 0$ [2]. Different choices of ordering would have different consequences for the theory of quantum gravity. Some orderings make the Wheeler-DeWitt a covariant equation and others make the Hamiltonian and other operators self-adjoint.

The only thing that can be done is to choose some ordering and study if the solutions of the equation *make sense*. *Making sense* in this context means to verify the consistency of solutions with some conditions imposed on the theory. This procedure is obscured by the fact that in the semi-classical approximation the operator ordering is irrelevant[48]. In the beginning of this chapter we use the ordering $i = -1$, $j = k = 0$ to explore the relation between tunnelling solutions and inflation. Wilthsire and Kontoleon studied the relations between the no-boundary and tunnelling wave functions, and several choices of factor ordering for a closed FRW model with a scalar field. They found that although the tunnelling wave function was consistently defined only for particular choices of factor ordering, the no-boundary wave function may be generically defined. The boundary conditions issue of quantum cosmology is the subject of the next section.

4.4 Boundary Conditions

It is important to understand that the Wheeler-DeWitt equation no more resolves the issue of quantum evolution of the universe, than the Schrödinger equation for any quantum system. The equation only evolves the states, it doesn't give us one [2]. What we mean is that even if the problem of time discussed earlier was solved or absent in some way we would still have to select some initial conditions for the wave function of the universe. It was initially hoped that a unique solution for the Wheeler-DeWitt equation would be found based purely on mathematical consistency [49]. It is now known that we must impose boundary conditions on wave function to select specific solution. The problem is that in quantum gravity there are no natural boundary conditions based physical grounds arising from symmetries. Hence, any choice must be imposed as a separate, fundamental physical law. There is a handful of different proposals for initial conditions. We shall mention the most discussed ones.

4.4.1 No-Boundary Proposal

The no-boundary proposal is of topological nature and it is based on the Euclidean path integral formulation of the wave function,

$$\Psi\left[h_{ij}, \Phi, \Sigma\right] = \int D(g_{\mu\nu}, \phi) e^{-S[g_{\mu\nu}, \phi]}. \tag{4.45}$$

where S is the classical action and $D(g_{\mu\nu}, \phi)$ is the measure in phase space[47]. In general, the integral cannot be solved exactly and we must use *stationary phase* approximations. The proposal then has two assumptions:

- The Euclidean form of the path integral is fundamental and the Lorentzian structure of space-time emerges when the stationary point of the phase are complex.
- Integration is carried over metrics and fields with one boundary only (The

present universe), so no *initial* boundary is present.

In the simplest model, at small radii, the main contribution is given by half of the Euclidean 4-sphere. At large radii the main contribution is given by the de Sitter, which is the analytic continuation of the Euclidean 4-sphere. The two geometries are matched by a 3-geometry. This situation is depicted in figure 4.2.

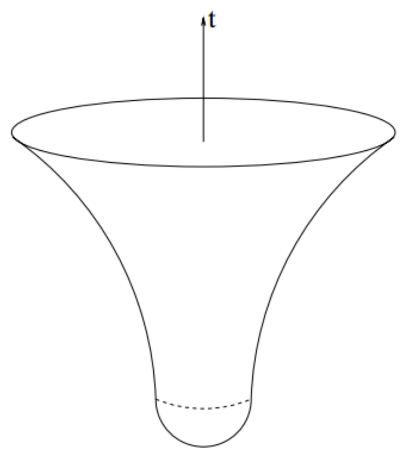

Figure 4.2: Graphic representation of the Hartle-Hawking proposal[51].

We can see that there is no singular boundary in the past. For the model represented by equation (4.44), in the no-boundary proposal we find the wave function[50]

$$\psi_{\text{N-B}} = \left(a^2 V(\phi) - 1\right)^{-\frac{1}{4}} \exp\left(\frac{1}{3V(\phi)}\right) \cos\left(\frac{\left(a^2 V(\phi) - 1\right)^{\frac{3}{2}}}{3V(\phi)} - \frac{\pi}{4}\right) \tag{4.46}$$

We should note that this no-boundary wave function is real. This is a consequence of the Euclidean path integral; even if complex metrics contribute they should do so in complex-conjugate pairs. Hence, the result is real. Alternative boundary conditions may directly give a complex wave function, being of the form exp(iS) in the semi-classical approximation. This is achieved by the tunnelling proposal[40].

4.4.2 Tunnelling Proposal

The tunnelling proposal comes from the work of Alexander Vilenkin[43, 44]. It is is most easily being formulated in mini-super-space. It states that the wave function consists of outgoing modes. More generally, it states that it consists solely of outgoing modes at singular boundaries of super-space (except the boundaries corresponding to vanishing three-geometry)[40]. But since there is no external evolution parameter it is necessary to define what *outgoing* means. This is possible using equation (4.32) and defining a probability current in the Klein-Gordon sense[37]

$$\mathbb{J} = i \int \Psi^* \left[h_{ij}\right] \left(G_{ijkl} \frac{\overrightarrow{\delta}}{\delta h_{kl}} - \frac{\overleftarrow{\delta}}{\delta h_{kl}} G_{ijkl} \right) \Xi \left[h_{ij}\right] D(h). \tag{4.47}$$

which is in fact conserved. In the mini-super-space approximation this becomes

$$\mathbb{J} = \frac{i}{2} \left(\psi^* \nabla \psi - \psi \nabla \psi^* \right). \tag{4.48}$$

A WKB solution of the form $C \exp(iS)$ leads to $\mathbb{J} = -|C| \nabla S$. Then, the tunnelling proposal implies that this current must point outwards at singular a and ϕ. If the wave function were real (as is the case in the no-boundary proposal), the current would vanish. Same as before, for our Wheeler-DeWitt equation we find that

$$\psi_{\mathrm{T}} = \left(a^2 V(\phi) - 1\right)^{-\frac{1}{4}} \exp\left(-\frac{1}{3V(\phi)}\right) \exp\left(-\frac{i\left(a^2 V(\phi) - 1\right)^{\frac{3}{2}}}{3V(\phi)}\right). \tag{4.49}$$

4.4.3 No-boundary Versus Tunnelling

Comparing equations (4.46) and (4.49) we see that both approaches lead to different wave functions. An important difference is that whereas the tunnelling condition is imposed in the oscillatory regime of the wave function, the no-boundary condition is implemented in the Euclidean regime; the oscillatory part of the wave function is then found by an analytic continuation. This leads in the above example to the crucial difference between $\psi_{\text{N-B}}$ and ψ_{T} that the tunnelling solution contains a factor $\exp(-1/3V(\phi))$, whereas the no-boundary solution has a factor $\exp(1/3V(\phi))$. If we ask for the probability of inflation (in the region where this equations are valid) in the sense of equation (4.32), we see that the tunnelling solution favours large values of ϕ, as would be needed for inflation. Therefore this approach seems to predict inflation. On the other hand, the no-boundary condition seems to prefer small values of ϕ and therefore seems to predict no inflation. Since inflation is needed to fix problems in classical cosmology, it seems natural to prefer the tunnelling solutions over the Hartle-Hawking proposal.

Chapter 5

Conclusions

We stated initially that canonical quantum gravity is and important candidates for providing a fundamental description of the universe. Although many open problems exist in the formulation of the subject as we have mentioned, we hope that we have shown that potential for such programme to achieve this goal. In particular, that, under certain conditions, a reliable connection between classical observations and quantum predictions may be made. We provided several of these connections in Chapter 4: *Applications, Issues and Predictions of the Wheeler-DeWitt Equation* for some specific examples. The principle part of the thesis, however, was concerned with the foundations on which such constructions were laid. That is, with the derivation of this approach to quantum gravity.

We began in Chapter 2: *Classical Cosmology* by presenting a basic synthesis of the landscape of classical cosmology for the FRW model. We did this for two reasons: First, the majority of applications of quantum gravity are made within this model. Second, having a reference of the classical theory makes the interpretation of the quantum theory easier.

A detailed derivation of the Wheeler-DeWitt equation was the subject of chapter 3. By decomposing the space-time manifold into a set of space-like hyper-surfaces it was possible to obtain a Hamiltonian description general relativity. The dynamics of the system were then found to be characterized by two constraints: the momentum and Hamiltonian constraints. It was shown that these constraints may be identified with the generators of surface deformations on three dimensional hyper-surfaces and the requirement that general relativity if invariant under diffeomorphism. We then proceeded with the quantization technique introduced by Dirac. Such technique is the subject of the appendix. The constraints were promoted to operator equations, acting on a wave functional, Ψ. We saw how the Hamiltonian constraint, $\hat{H}\Psi = 0$, becomes the central equation of quantum cosmology. Known as the Wheeler-DeWitt equation, it governs the dynamics of the quantum system. It is a second order functional differential equation defined on the super-space which is the phase space of general relativity: an infinite dimensional space of Euclidean 3-metrics and scalar matter fields. This infinite-dimensionality makes the system almost impossible to work with. This is a reason why the mini-super-space approximation is so common. This approximation gets rid of the infinite-dimensionality and leaves us with a space of approximately spatially homogeneous and isotropic 3-metrics and scalar fields. We found that the Wheeler-DeWitt equation lacks an external time parameter in the theory. The main result of this chapter is the equation (3.61).

We started chapter 4 by applying the general Wheeler-DeWitt equation to the FRW space-time to obtain equation (4.6). We used the result to show that there is a relation between tunnelling solutions of the Wheeler-DeWitt equation and the inflationary scenario of cosmology for the universes considered in chapter 2. Although such connections constitute a motivation for the canonical quantum gravity programme, we immediately turned our attention to the main issues that come with such theory. The first one was the problem of time. The concept of time in standard quantum mechanics is based on the existence of an external time parameter. the Wheeler-DeWitt equation doesn't have this external parameter, the question arises as to how to formulate a notion of evolution in a quantum theory of a re-parametrization invariant system. We reviewed the three main approaches to such problem and used consistently the initial example to illustrate the consequences of each approach. We saw that both *Time Before Quantization* and *Time after Quantization* tried to obtain a Schrödinger-like equation in which the time evolution is carried by an internal parameter. We showed that the main problem is that the choice of this internal parameter is not unique and reproduces inequivalent theories. The third approach was the *timeless option*. We presented how this option takes the view that time is not fundamental and that measurements of quantities in the quantum theory can only be made in terms of conditional probabilities. This approach seems to be the most least problematic, but it requires a major separation from the traditional interpretations of a quantum theory. We made emphasis on how the many-worlds interpretation of quantum mechanics becomes a necessity of the timeless option.

We also studied two more problems of the quantum theory of gravity, namely, the operator ordering and the boundary conditions. We presented an argument to show that the operator ordering problem is unavoidable in the Dirac quantization scheme. In the boundary conditions problem we presented two different proposals (no-boundary and tunnelling) in the context of the FRW model. We compared them in the semi-classical approximation and saw that, while the no-boundary proposal is more geometrically pleasing, Vilenkin's has the most desirable qualities since it predicts inflation.

Overall, we have shown that although the construction of traditional quantum cosmology, suffers from some fundamental issues in its definition, combined with the no-boundary or tunnelling proposals, it is seen have successes such as the prediction for sufficient inflation. In doing so we have provided a good, self-contained, introduction to the main ideas behind the derivation and implementation of the canonical quantum gravity programme.

Appendix A: Canonical Quantization of Constrained Systems

.0.4 Quantization of Unconstrained Systems

The term **Quantization** refers to to the procedure that has to be followed in order to obtain a quantum mechanical version of a physical system from its classical description. In particular, canonical quantization refers Dirac's procedure. His recipe starts with the Hamiltonian of the classical system. Lets consider a system with finite degrees of freedom, phase space variables (q_i, p^i) with $i = 1, \ldots, n$ and

$$\begin{aligned} \dot{q}_i &= \{q_i, H\} \\ \dot{p}^i &= \left\{p^i, H\right\}. \end{aligned} \tag{1}$$

with Hamiltonian $H = H(q,p)$ and canonical algebra $\{q_i, p^j\} = \delta_i^j$. Dirac's canonical programme is as follows:

- Phase space variables (q_i, p^i) are promoted to operators $(\hat{q}_i, \hat{p}^i)$ that act on vectors $|\psi\rangle \in \mathbb{V}$ of a Hilbert space $\mathbb{V}$.

- The operator algebra is obtained from classical algebra

$$\left\{q_i, p^i\right\} \to -i\left[\hat{q}_i, \hat{p^i}\right], \tag{2}$$

  where we have set $\hbar = 1$ in the interest of simplicity.

- Finally, evolution of the states $|\psi\rangle$ is governed by the Schrödinger equation

$$i\frac{\partial}{\partial t}|\psi\rangle = \hat{H}|\psi\rangle \tag{3}$$

  where the Hamiltonian operator is $\hat{H} = H(\hat{q}, \hat{p})$.

The harmonic oscillator is the typical example

.0.5 Hamiltonian Formulation of Constrained Systems

Let $L(q_i, \dot{q}_i)$ be the Lagrangian of some physical system (which does not depend on time explicitly). As we know, the equations of motion arise from the variational principle

$$\delta S = \delta\left(\int_{t_1}^{t_2} L(q_i, \dot{q}_i)dt\right) = 0. \tag{4}$$

Such equations are, obviously, the Euler-Lagrange equations

$$\frac{\partial L}{\partial q_i} = \frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i}. \tag{5}$$

If we introduce the conjugate momenta

$$p^i = \frac{\partial L}{\partial \dot{q}_i} \tag{6}$$

via a Legendre transformation we get the Hamiltonian (using Einstein's summation convention)

$$H(q_i, p^i) = p^i \dot{q}_i(p^i) - L(q_i, \dot{q}_i(p^i)). \tag{7}$$

Calculating the variation of the Hamiltonian we can see that it depends only on the phase space variables (q_i, p^i). If all the canonical variables are independent (meaning that al the velocities can be solved in term of the positions and momenta q_i, p^i), the equations of motion obtained by applying the variational principle to the new action

$$S = \int_{t_1}^{t_2} \left(p^i \dot{q}_i(p^i) - H(q_i, p^i)\right) dt. \tag{8}$$

are the Hamiltonian equations

$$\begin{aligned} \dot{q}_i &= \frac{\partial H(q_i, p^i)}{p^i} \\ \dot{p}^i &= -\frac{\partial H(q_i, p^i)}{\dot{q}_i}. \end{aligned} \tag{9}$$

In general, if we define the Poisson bracket for two different functions A and B of the phase space as

$$\{A, B\} = \frac{\partial A}{\partial q_i}\frac{\partial B}{\partial p^i} - \frac{\partial B}{\partial q_i}\frac{\partial A}{\partial p^i}, \tag{10}$$

the evolution of any function f of the phase space can be written as

$$\dot{f} = \{f, H\}. \tag{11}$$

In particular we recover equation (1). Up to this point, having put the theory in terms of the Poisson algebra, the quantization procedure described in the last section can be applied without changing it. But, if the variables are NOT all independent, there must be relations of the of the form $\phi_m(q,p) = 0$ with $m = 1, \ldots, M$ called **primary constraints**. In this case we call the Lagrangian **singular**. The singularity condition involves the determinant of the Jacobian of the transformation between $\dot{q}_i$ and p^i.

$$det \left(\frac{\partial p^i}{\partial \dot{q}_j} \right) = det \left(\frac{\partial^2 L}{\partial \dot{q}_j \partial \dot{q}_i} \right) = 0. \tag{12}$$

In order to get Hamilton equations of motion when the Lagrangian is singular we must solve the problem of finding the extrema of the action functional with constraints. This is achieved by using Lagrange multipliers. So the variational principle becomes

$$S = \int_{t_1}^{t_2} \left(p^i \dot{q}_i(p^i) - H(q_i, p^i) - \lambda^m \phi_m \right) dt \tag{13}$$

where the λ^m are the Lagrange multipliers. Caculating the variation of the action with respect to q_i, p^i and λ^m we find the new equations of motion

$$\begin{aligned} \dot{q}_i &= \frac{\partial H}{p^i} + \lambda^m \frac{\partial \phi_m}{p^i} \\ \dot{p}^i &= -\frac{\partial H}{\dot{q}_i} - \lambda^m \frac{\partial \phi_m}{q_i}, \end{aligned} \tag{14}$$

and, on top of that we must have

$$\phi_m \approx 0. \tag{15}$$

Now, equation (15) has a squiggly equal for a very important reason. The constraints have to be set to zero but only in final solutions, that is, only **after calculating Piosson brackets**. The argument is that its derivatives don't necessarily vanish. Dirac introduced this notation and called quantities joined by the squiggly lines *weakly equal*. We can redefine the Hamiltonian as

$$H^* = H + \lambda^m \phi_m. \tag{16}$$

Clearly, both Hamiltonians are weakly equal $H \approx H^*$and the equations of motion take the similar form

$$\begin{aligned} \dot{q}_i &= \frac{\partial H^*}{p^i} \\ \dot{p}^i &= -\frac{\partial H^*}{\dot{q}_i}, \end{aligned} \tag{17}$$

with $\phi_m \approx 0$. Using weak identities we can prove that the equations (17) are equivalent to those in (9). In fact, we get

$$\begin{aligned} \dot{q}_i &= \{q_i, H\} + \lambda^m \{q_i, \phi_m\} + \phi_m \{q_i, \lambda^m\} \\ \dot{p}^i &= \left\{p^i, H\right\} + \lambda^m \left\{p^i, \phi_m\right\} + \phi_m \left\{p^i, \lambda^m\right\}. \end{aligned} \tag{18}$$

With equation (15) it is easy to see the equality between (9) and (18). The last term is zero in the latter. Same as before, the evolution of functios of the phase space is given by

$$\dot{f} = \{f, H^*\} = \{f, H\} + \lambda^m \{f, \phi_m\}. \tag{19}$$

For the sake of consistency of the system's equations of motion, the primary constraints must be preserved in time, that is

$$\dot{\phi}_m = \{\phi_m, H^*\} = \{\phi_m, H\} + \lambda^{m'} \{\phi_m, \phi_{m'}\} \approx 0. \tag{20}$$

From the last relation exactly 4 things could happen:

1. We get a tautology ($0 = 0$).
2. We get an expression for the Lagrange multipliers.
3. We get new relations $\tilde{\phi}_{\tilde{m}} \approx 0$ with $\tilde{m} = 1, \ldots, \tilde{M}$ that are independent from the primary constraints. These new relations are called secondary constraints.
4. We get some mathematical inconsistency.

If 1. or 2. occurs, the process of constraints conservation ends.If 3. occurs, we must preserve the secondary constraints and get one of the three options mentioned (loop the process) and we finish when no more constraints can be obtained. If 4. occurs, the theory must be discarded. In this case the Lagrangian is not a *good* Lagrangian in the sense that it doesn't represent a valid description of a physical system. At the end of the process we wind up with $M + \tilde{M}$ constraints. However, we won't make distinction between primary and secondary constraints and we'll set the total number of constraints to M (primary and secondary). It should be noted that if we define a new **extended** Hamiltonian

$$\tilde{H} = H + \lambda^m \phi_m \tag{21}$$

where m runs over the total number of constraints, the new equations of motion, coming from a new extended variational principle, must be

$$\begin{aligned} \dot{q}_i &= \left\{ q_i, \tilde{H} \right\} \\ \dot{p}^i &= \left\{ p^i, \tilde{H} \right\}. \end{aligned} \tag{22}$$

The time evolution for any function in the phase space is

$$\dot{f} = \left\{ f, \tilde{H} \right\}. \tag{23}$$

It is important to point out that with H^* we can recover the original Euler-Lagrange of the Lagrangian description but with $\tilde{H}$ this is not possible. However, as we'll see in a moment the physics depicted by both Hamiltonians are equivalent and for that reason we'll use the extended Hamiltonian for the forthcoming discussions. As a consequence of the time preservation of the constraints we get a condition on the Lagrange multipliers given by the equation.

$$\left\{\phi_m, \tilde{H}\right\} + \lambda^{m'}\Theta_{mm'} \approx 0, \tag{24}$$

where $\Theta_{mm'} \approx \{\phi_m, \phi_{m'}\}$. We can think of $\Theta_{mm'}$ as a $M \times M$ matrix; and the objects $\left\{\phi_m, \tilde{H}\right\}$ and $\lambda^{m'}$ as components of vectors of dimension M. With such image we can propose a general solution to the system of equations

$$\lambda^m = \Xi^m + \Pi^m, \tag{25}$$

where $\Xi^m(q,p)$ is a particular solution of the equation $\Xi^m \{\phi_m, \phi_{m'}\} \approx -\left\{\phi_{m'}, \tilde{H}\right\}$. On the other hand, $\Pi^m(q,p)$ is a vector in $Ker(\Theta)$. Now, if Π^m_g with $a = 1, \ldots, G$ is a basis for $Ker(\Theta)$, then $\Pi^m_g = z^g\Pi^m_g$, where z^g are arbitrary coefficients. Having this in mind we can write

$$\tilde{H} = H + \Xi^m\phi_m + z^g\Pi^m_g\phi_m = H' + z^a\phi_a; \quad \text{with } \phi_a = \Pi^m_a\phi_m. \tag{26}$$

Clearly, the number of constraints ϕ_a is equal to $dim(Ker(\Theta))$. Again, the time evolution of functions is given by

$$\dot{f} = \{f, H' + z^a\phi_a\}. \tag{27}$$

By construction we have the weak identities $\{H', \phi_m\} \approx= 0$ and $\{\phi_a, \phi_m\} \approx 0$. The quantities whose Poisson bracket with all the constraints is weakly zero are called **first class constraints** (FCCs). Hence, we have found G first class constraints and $R = M - G$ **second class constraints** (SCCs). Π^j_a can be thought as a projector that extracts first class constraints from the complete set. We shall denote the second class constraints with χ_r, $r = 1, \ldots, R$. It is clear that the dimension of the rank of Θ is R. The way the elements of Θ are arranged depends on the way the constraints ϕ_m are listed. Nonetheless, physics cannot depend on an arbitrary label. Then, we can reorder the constraints in a useful manner. If we choose $\Pi_a^j = \delta_{a+R}^j$ we get a new set of $\tilde{\phi}_{mm'}$, where $\chi_r = \tilde{\phi}_r$ would be the first R constraints and $\phi_a = \delta_{a+R}^j \tilde{\phi}_j$ are the A last ones. In terms of our new order the matrix $\tilde{\Theta}$ is

$$\tilde{\Theta}_{=} \left(\begin{array}{cc} (\Omega_{rr'})_{R\times R} & 0_{R\times G} \\ 0_{G\times R} & 0_{G\times G} \end{array} \right). \tag{28}$$

with $\Omega_{rr'} = \{\chi_r, \chi_{r'}\}$. The zero matrices in equation (28) come from terms of the form $\{\phi_a, \bullet\}$. Dirac proved that $det(\Omega)$ is never zero so we can find its inverse. Then the number SCCs must be even since every skew-symmetric, hollow matrix of odd size has determinant zero. Finally, we obtain an expression for the time evolution

$$\dot{f} = \{f, H\} \{f, \chi_{r'}\} \Omega^{r's'} \{\chi_{s'}, H\} + z^a \{f, \phi_a\}. \tag{29}$$

At this point we define the **Dirac bracket** $\{\}^*$

$$\{A, B\}^* = \{A, B\} - \{A, \phi_j\} \Theta^{jj'} \{\phi_{j'}, B\}. \tag{30}$$

Equation (29) becomes

$$\dot{f} = \{f, H + z^a \phi_a\}^*. \tag{31}$$

The Dirac bracket has the same properties as the Poisson bracket with the added characteristic that it is identically zero when evaluated between a function of the phase space and any constraint of the second class.

.0.6 First Class Constraints and Gauge Transformations

As seen in the last section, the *complete* Hamiltonian contains arbitrary functions z^a. This implies that the trajectory $f(t)$ of a function f in the phase space with time evolution governed by equation (31) isn't unequivocally since we could choose different functions z^a. This lead us to propose that if the evolution of two quantities f and f' depends on the choice of z^a, then they must be physically equivalent. To see that they are in fact related by a gauge transformation lets consider f with initial condition $f_0 = f(t = t_0)$ and lets choose $z^a = z_1^a$. After an infinitesimal time δt we have

$$\begin{aligned} f(t_0 + \delta t) &= f_0 + \dot{f}\delta t + O(\delta t^2) \\ &= f_0 + \{f, H'\}\,\delta t + z_1^a\,\{f, \phi_a\}\,\delta t + O(\delta t^2). \end{aligned} \tag{32}$$

If we choose $z^a = z_2^a$ instead we get

$$f'(t_0 + \delta t) = f_0 + \{f, H'\}\,\delta t + z_2^a\,\{f, \phi_a\}\,\delta t + O(\delta t^2). \tag{33}$$

Subtracting both equations we find

$$\delta f = f(t_0 + \delta t) - f'(t_0 + \delta t) = (z_1^a - z_2^a)\,\delta t = \{f, \varepsilon^a \phi_a\}\,. \tag{34}$$

ε^a is an arbitrarily small quantity. Then, f and f' are related by a gauge transformation given by (34). Such equation tells us that **first class constraints are gauge transformation generators**. Now, quantities that physically relevant (what we call observables) are invariant under such transformations and must satisfy $\{f, \phi_a\} = 0$. By construction we know that H', SCCs and Poisson brackets of FCCs are observables. In fact, the set of FCCs constitute a closed algebra, which is compatible with their as generators of the gauge group. The presence of FCCs implies that we are using more degrees of freedom than those that are really needed to describe the physical system. However, sometimes is useful so reduce those degrees of freedom by gauge fixing with the objective of obtaining a set of only SCCs.

.0.7 Quantization

Up until now we have talked about the Hamiltonian formulation of classical singular systems. The next step is construct a quantum version of such systems. When the the theory is singular the procedure outlined at the beginning of the appendix have to be modified to include the effects of the constraints. We'll obtain two different recipes, one for when the system has only FCCs and another one for when it has SCCs. Although, for both procedures the starting point is the same:

- Phase space variables (q_i, p^i) are promoted to operators $(\hat{q}_i, \hat{p}^i)$ that act on vectors $|\psi\rangle \in \mathbb{V}$ of a Hilbert space $\mathbb{V}$.
- The operator algebra is obtained from classical algebra

$$\left\{q_i, p^j\right\} \to -i\left[\hat{q}_i, \hat{p}^i\right]. \tag{35}$$

.0.7.1 Systems with FCCs

The FCCs are gauge transformation generators in the classical version and we would like the corresponding quantum version to be invariant under these transformations in certain representation $\hat{\phi}_a$ generated by the assignment $(q_i, p^i) \to (\hat{q}_i, \hat{p}^i)$. So, we will require the physical states $|\psi\rangle_{phis}$ to be invariant under the transformation, that is, $e^{i\varepsilon^a\hat{\phi}_a}|\psi\rangle_{phis} = |\psi\rangle_{phis}$. From this we get the condition

$$\hat{\phi}_a|\psi\rangle_{phis} = 0. \tag{36}$$

Equation (36) is the third step in our recipe. The final step is to require that the evolution of the physical states has to be governed by the Schrödinger equation

$$i\frac{\partial}{\partial t}\left|\psi\right\rangle_{phis} = \hat{\tilde{H}}\left|\psi\right\rangle_{phis} = \hat{H}'\left|\psi\right\rangle_{phis} + z^a\hat{\phi}_a\left|\psi\right\rangle_{phis} = \hat{H}\left|\psi\right\rangle_{phis}. \tag{37}$$

Here $\hat{H}$ is the operator we get from the classical H since H' contains only FCCs which annihilate the physical states.

.0.7.2 Systems with SCCs

In this case, SCCs are not gauge transformation generators, so when they act on states $|\psi\rangle$ they won't reduce the phase space. In consequence, for any representation of the SCCs it must happen that

$$\hat{\chi}_r = 0 \tag{38}$$

This way the relation $\hat{\chi}_r\left|\psi\right\rangle = 0$ holds without imposing conditions on the phase space. But if we consider the Poisson bracket we get

$$[\hat{\chi}_r, \hat{\chi}_{r'}]\left|\psi\right\rangle = \hat{\chi}_r, \hat{\chi}_{r'}\left|\psi\right\rangle - \hat{\chi}_{r'}\hat{\chi}_r\left|\psi\right\rangle. \tag{39}$$

The left hand side is never zero but the right hand side is identically zero. To avoid this contradiction we redefine the operator algebra using the Dirac bracket.

$$\left\{q_i, p^i\right\}^* \to -i\left[\hat{q}_i, \hat{p}^i\right], \tag{40}$$

Finally, the evolution of quantum states is governed by

$$i\frac{\partial}{\partial t}\left|\psi\right\rangle_{phis} = \hat{\tilde{H}}\left|\psi\right\rangle_{phis} = \hat{H}\left|\psi\right\rangle_{phis}. \tag{41}$$

Since, classically, $\hat{H}$ and H' contain SCCs. If the theory has both FCCs and

SCCs, we could still use equation (40) to define the operator algebra because the Dirac bracket between a FCC and any function on the phase space is equal to their Poison bracket. In fact, if f is first class quantity and g is any other function we have

$$\{f, g\}^* = \{f, g\} - \{f, \chi_r\} \Lambda^{rr'} \{\chi_{r'}, g\} = \{f, g\} . \tag{42}$$

Here we have made a rather short review of the quantization of constrained systems. Our objective was to give a reference frame in which the methods used in 3.2 can be understood to some extent. Much was overlooked, in particular, the generalization to infinite degrees of freedom (although is straightforward). For a more complete discussion on the subject of canonical quantization see for example [52], [53] or [54]; sources that were used in the development of this section.

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