We develop a first order formalism for the quantization of gravity. We take as canonical variables both the induced metric and the extrinsic curvature of the \((d-1)\)-dimensional hypersurfaces obtained by the foliation of the \(d\)-dimensional spacetime. After solving the constraint algebra we use the Dirac formalism to quantize the theory and obtain a new representation for the Wheeler-DeWitt equation, defined in the functional space of the extrinsic curvature. We also show how to obtain several different representations of the Wheeler-DeWitt equation by considering actions differing by a total divergence. In particular, the intrinsic and extrinsic time approaches appear in a natural way, as do equivalent representations obtained by functional Fourier transforms of appropriate variables. We conclude with some remarks about the construction of the Hilbert space within the first order formalism.
1. Introduction

One of the long standing problems of physics is the quantization of the gravitational field. Although this question is almost as old as general relativity, it has been mostly in the last thirty years that many attempts to obtain a consistent theory of quantum gravity have been developed [1]. In fact, looking through the literature, one soon realizes the various schools of thought that mainly reflect personal ways of tackling the problem, although there is a traditional division in two groups; on one side stands the particle physicist's way of treating the graviton as the bearer of quantum fluctuations of the gravitational field around a classical background, the goal being the construction of a renormalizable -or even finite- S-matrix that would describe the interactions of the gravitons between themselves and other matter fields present. This is known as the covariant method. On the other side stands the general relativist's method with its emphasis on geometry, topology and spacetime structure and its conceptual independence on the asymptotic structure at infinity which, in principle, is applicable to both closed and open universes. This is known as the canonical method. The first method is more adequate for calculations of scattering amplitudes in asymptotically flat Euclidean spaces, while the second method is concerned with the strong non-linear effects that appear near a spacetime singularity or at the Planck scale.

This work was originally motivated by the important role that higher-order curvature terms are believed to play when studying gravity at distances close to the Planck length. These modifications of pure gravity seem to be justified even in light of string theories, where the "low energy" effective action naturally has higher-order curvature terms [2]. In
fact, we were particularly interested in studying the effects of topological terms such as
the Chern-Simons [3] terms in (2 + 1) -dimensions and the Euler-Gauss-Bonnet (EGB)
combination in d -dimensions (d > 4) on the Wheeler-DeWitt approach to the wave
function of the universe [4]. Nevertheless, as we will see below, the construction of a
Hamiltonian formalism for the quantization of these theories is far from trivial.

As an illustration, let us consider the EGB combination for arbitrary d > 4 . Con-
trary to the 4 -dimensional case, the EGB is not a topological invariant and thus can
be considered as a viable quadratic curvature action with the unique property amongst
such actions that its variation does not involve explicit derivatives of the curvature. If we
follow the usual canonical formalism, it is best to adopt the method of Arnowitt, Deser
and Misner (ADM) [5], and consider a decomposition of spacetime into a one-parameter
family of space-like hypersurfaces by writing the d dimensional line element as

\[
d s^2 = -N^2 dt^2 + h_{ij}(dx^i + N^i dt)(dx^j + N^j dt)
\]

where \( N \) and \( N^i \) are known as the lapse function and shift vector, respectively. The
tensor \( h_{ij} \) is the induced metric of the space-like hypersurface and the indices \( i,j,... \)
run from 1 to \( d - 1 \) [5]. In what follows, greek indices will cover the whole spacetime.

Quantities built from \( h_{ij} \) have a tilde superscript.

If we write the Lagrangian density as

\[
\mathcal{L} = k^{-1} R + \alpha(R_{\mu\nu\rho\sigma}R^{\mu\nu\rho\sigma} - 4R_{\mu\nu}R^{\mu\nu} + R^2)
\]

we obtain, after a tedious calculation, the action in ADM form
\[ I = \int dt d^{d-1}z \sqrt{h} \left\{ k^{-1}(\text{tr} K^2 - K^2 + \tilde{R}) + \alpha \left[ (2\text{tr} K^4 - (\text{tr} K^2)^2 + 2K^2\text{tr} K^2 + \right. \right. \]
\[ - \frac{8}{3} K\text{tr} K^3 - \frac{1}{3} K^4 \left. \left. \right) + (-4\tilde{R}_{ijkl}K_{ij}^4 K_{kl}^4 - 8\text{tr}(K^2 \tilde{R}) - 2\tilde{R}K^2 + \right. \right. \]
\[ + 2\tilde{R}\text{tr} K^2 + 8K(\text{tr} K \tilde{R}) + (\tilde{R}_{ijkl}K_{ij}^4 K_{kl}^4 - 4\tilde{R}_{ij} K_{ij}^2) \right\} + \text{s.t.} \]  

where, \( \text{tr}(K \tilde{R}) = K_{ij} \tilde{R}_{ij} \); \( K^2 = (h^{ij} K_{ij})^2 \); \( \text{tr}(K^2 \tilde{R}) = \tilde{R}_{sk} K^i s K_k^i \); \( \text{tr} K^4 = K_i^p K_p m K_m \); \( \text{tr} K^3 = K_i^j K^p K_{pi} \); \( \text{tr} K^2 = K_{ij} K^{ij} \). \( K_{ij} \) is the extrinsic curvature of the space-like hypersurface defined as the differential change in the unit normal projected into the surface, \( K_{ij} = -n_{j||i} \). The parallel bars denote covariant derivatives with respect to the full metric of spacetime.

Following the usual procedure, we should now obtain the canonical momenta \((\pi, \pi^i, \pi^ij)\) conjugate to the canonical variables \((N, N^i, h^ij)\) and then write the Hamiltonian in terms of the variables and the momenta. The reader can easily verify that, contrary to the Einstein-Hilbert case, the action has terms with \( K^4 \) and thus that \( \pi^ij \) has terms proportional to \( K^3 \). As it stands, we cannot write the Hamiltonian as being quadratic in the momenta. We then decided to treat \( K_{ij} \) as an independent variable by going to a first order formalism; the introduction of an extra canonical variable and its conjugate momentum could be useful in the construction of the correct Hamiltonian of theories with higher order terms in the curvature.

As a first step towards this final goal, we start with the simplest possible case: The construction of a first order formalism for Einstein gravity. As we will show, there is a rich structure to be explored by going to first order even in this apparently simple case. In fact, as it turns out, the theory is far from being trivial; we will have to deal with
the quantization of a theory with second class constraints having, as a guideline, the final equivalence between the first and the second order formalisms. The advantage of using a first order formalism comes from the choice of different representations that are possible, due precisely to the second class constraints. As it is well known [6], when quantizing a theory with second class constraints, one has to reduce the largest possible number of second class constraints into first class since the latter are the ones to be applied on the wave functional. The remaining second class constraints are to be treated as identities between quantum operators, thus providing a relation between different possible representations. We will explore this idea extensively in this work, and will show how the pairs of canonical variables and conjugate momenta \((h^{ij}, \pi_{ij})\) and \((K_{ij}, P^{ij})\) are related by the second class constraints and can be used to obtain different representations of the Wheeler-DeWitt equation. We will also show how different representations found previously in the literature can be derived naturally from the first order formalism.

The paper is organized as follows; in section 2 we develop the classical theory in first order form by building the total Hamiltonian, implementing the relevant constraints and by classifying them into first and second class. We show that the theory has \(d^2\) second class constraints but that \(d\) of those can be reduced to first class. We use the Dirac formalism [6] and construct the Dirac brackets in order to obtain the proper commutation relations between the variables. In section 3 we quantize the classical theory built in section 2. We show that once the commutation algebra is constructed we can have two possible representations of the Wheeler-DeWitt equation, where the wave functional may depend either on the metric or on the extrinsic curvature of the space-like hypersurface. (Actually,
things are not so simple. In order to obtain the correct commutation relations we have
to redefine the canonical variables. The pairs of variables that will furnish equivalent
representations are \((h^{ij}, \pi_{ij}^{\prime})\) and \((K_{ij}^{\prime}, P^{ij})\), where the prime denotes the new canonical
variable.) Section 3 ends with a discussion of several other representations that can be
obtained by the proper manipulation of the first order action via different integrations by
parts and the identification of the correct dynamical variables. We conclude in section
4 with a brief discussion on the construction of the Hilbert space within the first order
formalism and by summing up our results and remaining questions.

2. Constraint structure of gravity in first order form

By using the ADM decomposition of spacetime as in eq. (1.1), we can write the Einstein-
Hilbert action

\[
I[g^{\mu\nu}] = \int d^d x (-g)^{1/2} g^{\mu\nu} R_{\mu\nu}
\]

(2.1)
as,

\[
I[h^{ij}, K_{ij}, N, N'] = \int d^d x h^{1/2} [ -2h^{ij} K_{ij} - h^{ij} K_{ij} + N(\ddot{R} + K^2 - K_{ij} K^{ij}) \\
- 2N' (K_i^j - \delta_i^j K)_;,j - 2(N_i; - K_{ij} N^j);i ] .
\]

(2.2)

Note that we are taking both \(h^{ij}\) and \(K_{ij}\) as independent variables, which is equi-

valent to the use of the Palatini formalism. The last term is a surface term that can be

eglected since its variation vanishes. The dot indicates time derivatives, and the semi-
colon denotes covariant derivatives with respect to the metric of the hypersurface. We are

only considering vacuum closed spacetimes. The extension of this formalism to include

matter fields is straightforward.
In order to obtain the action familiar of the second order treatment [7], we have to use the definition of the connection in terms of the metric that, in the language of the ADM decomposition, is given by

\[ h^{ij} = 2K^{ij} + N^{(ij)} \]  

(2.3)

where the parentheses imply symmetrization of the indices. If we integrate the first term of (2.2) by parts and use (2.3), the action (2.2) becomes,

\[ I[h^{ij}, N, N'] = -2 \int_{\partial M} d^{d-1}x h^{1/2}K + \int d^d x N h^{1/2}[K_{ij}K^{ij} - K^2 + \tilde{R}] , \]  

(2.4)

where \( M \) is the \( d \)-dimensional manifold and \( \partial M \) its boundary. As it is well known in the literature [8], we must add the surface term appearing in (2.4) to the Einstein-Hilbert action (2.1) so that its variation with respect to \( h^{ij} \) will give Einstein’s equations.

Now we start the detailed study of the first order formalism. In order to build the Hamiltonian from the action (2.2), we first calculate the conjugate momenta to the variables \( N, N^i, h^{ij} \) and \( K_{ij} \),

\[ \pi_i = \frac{\partial L}{\partial \dot{N}^i} = 0 \]  

(2.5a)

\[ \pi^i = \frac{\partial L}{\partial \dot{N}^i} = 0 \]  

(2.5b)

\[ \pi_{ij} \equiv \frac{\partial L}{\partial \dot{h}^{ij}} = -h^{1/2}K_{ij} \]  

(2.5c)

\[ \pi^{ij} \equiv \frac{\partial L}{\partial \dot{K}_{ij}} = -2h^{1/2}h^{ij} \]  

(2.5d)

The Hamiltonian density is then given by

\[ \mathcal{H}_0 = h^{1/2}[-N(\tilde{R} + K^2 - K_{ij}K^{ij}) + 2N^i(K_i^j - \delta_i^j K)_{ij}] . \]  

(2.6)
The subscript 0 is a reminder that this is not the most general Hamiltonian of the theory.

Following Dirac [6], whenever we have relations of the kind \( \phi(q, p) = 0 \) (the primary constraints) the total Hamiltonian must include linear combinations of these constraints.

We thus define the total Hamiltonian density,

\[
H_T = \kappa_0 - \hbar^{1/2} \left[ \lambda^{ij} (\pi_{ij} + \hbar^{1/2} K_{ij}) + \omega_{ij} (P^{ij} + 2\hbar^{1/2} h^{ij}) + \lambda \pi + \lambda_i \pi_i \right]. \tag{2.7}
\]

\( \lambda, \lambda_i, \lambda^{ij} \) and \( \omega_{ij} \) are Lagrange multipliers that can, in principle, be functions of the canonical variables.

We can write the Hamilton's equations of motion using the Poisson brackets, \( \dot{g} = \{g, H_T\} \), where \( g \) is any function of the canonical variables and \( H_T \) is the total Hamiltonian. In order for the theory to be consistent classically, the constraints must be maintained by the time evolution of the system. In other words, their Poisson brackets with the total Hamiltonian must vanish. We use the notation weakly equal \( (\approx) \) to remind us of only using the constraints after calculating the brackets. The only non-zero Poisson brackets between the canonical variables are

\[
\{h^{ij}(x), \pi_{lm}(x')\} = \frac{1}{2} (\delta^i_l \delta^j_m + \delta^i_m \delta^j_l) \delta^d(x - x') \tag{2.8a}
\]

\[
\{K_{ij}(x), P^{lm}(x')\} = \frac{1}{2} (\delta^i_l \delta^j_m + \delta^i_m \delta^j_l) \delta^d(x - x') \tag{2.8b}
\]

(Of course, \( \{N, \pi\} \) and \( \{N^i, \pi_i\} \) are not zero but they will not be relevant, as we will see below.)

Note that Hamilton's equations for the canonical variables give,

\[
\dot{N} = \frac{\partial H_T}{\partial \pi} = \{N, H_T\} = -\hbar^{1/2} \lambda \tag{2.9a}
\]
\[ \dot{N}^i = \frac{\partial \mathcal{L}_T}{\partial \pi_i} = \{N^i, H_T\} = -\hbar^{1/2} \lambda^i \quad (2.9b) \]
\[ \dot{\lambda}^i_{ij} = \frac{\partial \mathcal{L}_T}{\partial \pi_{ij}} = \{\lambda^i_{ij}, H_T\} = -\hbar^{1/2} \lambda^i_{ij} \quad (2.9c) \]
\[ \dot{K}_{ij} = \frac{\partial \mathcal{L}_T}{\partial \mathcal{P}_{ij}} = \{K_{ij}, H_T\} = -\hbar^{1/2} w_{ij} \quad (2.9d) \]

From (2.9a) and (2.9b) we can see that \( N \) and \( N^i \) are arbitrary. The Poisson brackets of \( \pi \) and \( \pi^i \) with \( H_T \) will imply that the two terms in (2.6) are separately zero. They are called the secondary constraints, with \( N \) and \( N^i \) playing the role of Lagrange multipliers. We can thus discard \( N \) and \( N^i \) as canonical variables and consider \( \mathcal{H}_T \) without the last two terms.

Now we must calculate the Poisson brackets of all the constraints with \( H_T \). According to Dirac, we can obtain three possible results:

i) \( 0 \approx 0 \) which is trivial;

ii) \( \psi(q, p) \approx 0 \), i.e., we may obtain another condition on the canonical variables, independent of \( \lambda \) and \( w \), the secondary constraints. We must make sure that they are conserved in time in the same way as primary constraints and repeat the process until all consistency conditions are exhausted. As just mentioned, this is the case for \( \{\pi, H_T\} \) and \( \{\pi^i, H_T\} \);

iii) We may obtain equations for the Lagrange multipliers as functions of the canonical variables. This will turn out to be the case in our formalism. In principle [6], we should add to the solutions of the inhomogeneous equations in iii) the solutions of the associated homogeneous equations, (related to the eq. \( \{\phi_i, \mathcal{L}_0\} + u_m \{\phi_i, \phi_m\} \approx 0 \), where \( \phi_i \) is an abbreviation for the constraints), \( V_m \{\phi_i, \phi_m\} = 0 \), but in our case the coefficients \( V_m \) are all zero;
iv) It may not be possible to obtain any solution. The Lagrangian is inconsistent.

Writing the constraints as

\[ H_0 = -h^{1/2}(\mathbf{R} + \mathbf{K}^2 - K_{ij}K^{ij}) \approx 0 \]

\[ H_i = 2h^{1/2}(K_i^j - \delta_i^j K)_{ij} \approx 0 \]

\[ \phi_{ij}^1 = \pi_{ij} + h^{1/2}K_{ij} \approx 0 \]

\[ \phi_{ij}^2 = P_{ij} + 2h^{1/2}h^{ij} \approx 0 \]

we obtain for the Poisson brackets between all the constraints (the ' denotes a quantity evaluated at the point \( x' \))

\[ \{H_0, H'_i\} = \{H_0, H'_0\} = \{H_i, H'_j\} = 0 \] (2.10a)

\[ \{H_0, \phi_{ij}^1\} = -h^{1/2}[h_{ij}h^{cd}\delta(x - x'),ijd - \delta(x - x'),ij + + (\tilde{R}_{ij} + 2\mathbf{K}K_{ij} - 2K_i^kK_k^j)\delta(x - x')| - \frac{1}{2}H_0\delta(x - x')h_{ij} \] (2.10b)

\[ \{H_0, \phi_{ij}^2\} = 2h^{1/2}(K_i^j - h_{ij}K)\delta(x - x') \] (2.10c)

\[ \{H_i, \phi_{kl}^1\} = H_i h_{kl} \delta(x - x') + h^{1/2}[(K_{ik}\delta(x - x'))_i + + (K_{il}\delta(x - x'))_k - K_{kl;}\delta(x - x') + - (K_{kl}\delta(x - x'))_i - K_{kl}^m h_{kl} \delta(x - x')_m \] (2.10d)

\[ \{H_i, \phi_{kl}^{2}\} = -2h^{1/2}[h^{kl}\delta(x - x'),i - \frac{1}{2}(\delta_k^l h^{ij} + \delta_l^i h^{kj})\delta(x - x')_j \] (2.10e)

\[ \{\phi_{ij}^1, \phi_{kl}^1\} = -\frac{1}{2}h^{1/2}(K_{ij}h_{kl} - h_{ij}K_{kl})\delta(x - x') \] (2.10f)
\{\psi_{ij}^*,\psi^{i'2kl}\} = -\hbar^{1/2}(\delta_{ij}^{kl} - h^{kl}h_{ij}) \tag{2.10} \]

\{\phi_{ij}^*,\phi^{i'2kl}\} = 0 \tag{2.10h}

Note that there is no constraint that commutes with all others. Following Dirac's nomenclature, we call these second class constraints. Thus, all \(d^2\) constraints of the theory are second class. Here, the differences from the first and second order formalisms are evident; in the latter case all \(d\) constraints are first class and can be directly imposed on the wave functional in the quantization of the theory. In first order form more work must be done before we quantize.

We must first impose the constancy in time of the \(d^2\) second class constraints by putting their Poisson brackets with the total Hamiltonian weakly equal to zero. The results can be easily read out from eq.(2.10). From the brackets with the constraints \(\phi^1\) and \(\phi^2\) it is easy to verify that one obtains two equations expressing the Lagrange multipliers in terms of the canonical variables as

\[
\lambda_{ij} = -\hbar^{1/2}(2NK_{ij} - N_{i'j} - N^{ij}') \tag{2.11a}
\]

\[
w_{ij} = -\hbar^{1/2}[N(\ddot{R} + KK_{ij} - 2K_{m}^{m}K_{ij}) - N_{i'j} + N_{m;i}K_{j}^{m} + N_{m;j}K_{i}^{m} + N^{m}K_{ij;m}] \tag{2.11b}
\]

With the above values of \(\lambda_{ij}\) and \(w_{ij}\) we obtain Einstein's equations,

\[
\dot{K}_{ij} = \{K_{ij},H_T\} = w_{ij} \quad (G_{\mu\nu} \phi^\mu_{\alpha} \phi^\nu_{\beta} = 0) \tag{2.12a}
\]

\[
\dot{\lambda}^{ij} = \{\lambda^{ij},H_T\} = \lambda^{ij} \quad (g_{\mu\nu||\alpha} = 0) \tag{2.12b}
\]
\[ \dot{\pi}_{ij} = \{\pi_{ij}, H_T\} \quad (G_{\mu\nu} \perp_\alpha \perp_\beta = 0 \text{ and } g_{\mu\nu||\alpha} = 0) \quad (2.12c) \]

\[ \dot{p}_{ij} = \{p_{ij}, H_T\} \quad (g_{\mu\nu||\alpha} = 0) \quad (2.12d) \]

while the variation of the total Hamiltonian with respect to the Lagrange multipliers give

\[ \frac{\delta H_T}{\delta N} = 0 \Rightarrow \tilde{R} + K^2 - K_{ij} K^{ij} = 0 \quad (G_{\mu\nu} n^\mu n^\nu) \quad (2.12e) \]

\[ \frac{\delta H_T}{\delta N^i} = 0 \Rightarrow (K_i^j \delta_i^I K)_{;i} = 0 \quad (G_{\mu\nu} n^\mu \perp_\alpha = 0) \quad (2.12f) \]

\[ \frac{\delta H_T}{\delta \lambda^{ij}} = 0 \Rightarrow \pi_{ij} + h^{1/2} K_{ij} = 0 \quad (2.12g) \]

\[ \frac{\delta H_T}{\delta w_{ij}} = 0 \Rightarrow p_{ij} + h^{1/2} h^{ij} = 0 \quad (2.12h) \]

where \( G_{\mu\nu} \) is the Einstein tensor, the parallel bars denote covariant derivatives with respect to the full metric of spacetime and \( \perp_\alpha^\mu \) is the projector onto the hypersurface.

Also, the \( d \) remaining Poisson brackets with \( H_0 \) and \( H_i \) will not impose any restrictions on \( N \) and \( N^i \). This suggests that \( d \) out of the \( d(d - 1)/2 + d(d - 1)/2 + d \) second class constraints are first class, since there are \( d \) Lagrange multipliers that are not fixed by the dynamics [6].

The next step is then to reduce \( d \) of the \( d^2 \) second class constraints to first class by considering linear combinations of the second class constraints. We can do this by noting that the total Hamiltonian, which is a linear combination of the second class constraints, is automatically a first class constraint since its Poisson brackets with all constraints are weakly equal to zero. In order to obtain \( d \) first class constraints that are not integral out of \( H_T \) (the first class constraints are going to be applied on the wave function to generate a differential equation) we simply use the freedom in \( N \) and \( N^i \) (remember they are arbitrary) by choosing, respectively
i) \(N = \delta(x - x'); \ N^i = 0\)

\[
\vec{H}_0 = \hbar^{1/2}(R + K^2 - K_{ij}K^{ij}) + 2K^{ij}\pi_{ij} + (R_{ij} + KK_{ij} - 2K_p^jK_{pj})P_{i}^j - P_{i}^j (2.13a)
\]

ii) \(N = 0, \ N^i = \delta^i_a\delta(x - x')\)

\[
\vec{H}_a = 2\pi_{aij}^i - 2K_{ajti}^i P_{ti}^j - 2K_{aj}^i P_{ti}^j + K_{ij;a}^i P_{ti}^j (2.13b)
\]

In this way we obtain \(d\) first class constraints \((\vec{H}_0\) and \(\vec{H}_a\)) and are left with \(d(d - 1)\) independent second class constraints \((\phi_{ij}^1\) and \(\phi_{ij}^2\)). The latter will become strong equalities between quantum operators once we introduce the Dirac brackets (i.e. they will commute with every function of the canonical variables) [6],

\[
\{A(x), B(y)\} = \{A(x), B(y)\} - \int du dv \{A(x), \phi^\alpha(u)\}(C^{-1})_{\alpha\beta}(u, v)\{\phi^\beta, B(y)\} (2.14)
\]

where the matrix \(C^{\alpha\beta}_{ij}(kl) = \{\phi^i_j, \phi^k_l\}\) is built from the second class constraints only. In our case we obtain,

\[
(C^{-1})^{(ij)(kl)}_{(11)} = 0
\]

\[
(C^{-1})^{(kl)}_{(21)(ij)} = -(C^{-1})^{(kl)}_{(12)(ij)} = -\hbar^{-1/2}(\delta^{kl}_{ij} - \frac{1}{d-2}h_{ij}h^{kl})\delta(x - x')
\]

\[
(C^{-1})^{(ij)(kl)}_{(22)} = -\frac{1}{2}\hbar^{-1/2}(h_{ij}K_{kl} - h_{kl}K_{ij})\delta(x - x')
\]

With this prescription we eliminate the spurious variables that come from the second class constraints. In fact, we can now use these constraints to choose between two equivalent representations,

\[
\pi_{ij} = -\hbar^{1/2}K_{ij}; \ P_{ij}^i = -2\hbar^{1/2}h_{ij}
\]
since we now have $2^{ \frac{d(d-1)}{2} }$ independent canonical variables out of the $4^{ \frac{d(d-1)}{2} }$ original ones.

Let us start with the conventional pair $(h^{ij}, \pi_{ij})$:

The Dirac brackets are,

$$\{h^{ij}(x), h^{kl}(y)\}^* = 0$$

$$\{h^{ij}(x), \pi_{kl}(y)\}^* = (-\delta_{kl}^{ij} + \frac{1}{d-2} h^{ij} h_{kl}) \delta(x - y)$$

$$\{\pi_{ij}(x), \pi_{kl}(y)\}^* = \frac{\hbar^{1/2}}{d-2} (K_{ij} h_{kl} - h_{ij} K_{kl}) \delta(x - y) .$$

The two last brackets are telling us that $\pi_{ij}$ is not a good canonical variable (i.e., when passing to the quantum formalism we cannot identify $\pi_{ij}$ with $-i \frac{\delta h^{ij}}{\delta h_{ij}}$). We can easily find the correct variable to be $\pi'_{ij} = -\pi_{ij} + h_{ij} \pi$ with the two last brackets being now,

$$\{\pi'_{ij}(x), \pi'_{kl}(y)\}^* = 0$$

$$\{h^{ij}(x), \pi'_{kl}(y)\}^* = \delta_{kl}^{ij} \delta(x - y) .$$

With this choice, the $d$ first class constraints (eq.(2.13)) become

$$\hat{H}_a = 2\pi''_{aij} \approx 0 \quad (2.15a)$$

$$\hat{H}_0 = \frac{1}{2} \hbar^{-1/2} [h^{ik} h_{jl} + h^{il} h_{jk} - \frac{2}{d-2} h^{ij} h_{kl}] \pi'_{ij} \pi'_{kl} - h^{1/2} \tilde{R} \approx 0 \quad (2.15b)$$

These are the familiar super-momentum and super-Hamiltonian constraints for Einstein gravity. Thus this choice of variables reproduces the results obtained from the second order formalism as expected.
The other possible choice is the pair \((K_{ij}, P^{ij})\). Again, the Dirac brackets tell us that the variable \(K_{ij}\) is not the proper one. By introducing \(K'^{ij}_{ij} = \frac{1}{2}(K_{ij} + \frac{1}{d-3}h_{ij}K)\) we obtain,

\[
\{P^{ij}(x), P^{kl}(y)\}^* = \{K'^{ij}_{ij}(x), K'^{kl}_{kl}(y)\}^* = 0
\]

\[
\{K'^{ij}_{ij}(x), P^{kl}(y)\}^* = \delta^{kl}_{ij}(x - y)
\]

In order to express the first class constraints in eq. (2.13) in terms of these variables we must use the second class constraints to obtain

\[
\pi_{ij} = -(-2)^{\frac{d-4}{2}} P^{(d-3)^{-1}} K_{ij}; \quad h^{1/2} = (-2)^{\frac{d-4}{2}} P^{(d-3)^{-1}}
\]

\[
h'_{ij} = \left(\frac{4}{P}\right)^{(d-3)^{-1}} P^{ij}; \quad h_{ij} = \left(\frac{P}{4}\right)^{(d-3)^{-1}} P^{ij}
\]

where \(P = \det P^{ij}\) and \(P_{ij} = (P^{ij})^{-1}\).

With these substitutions, the constraint (2.13b) becomes,

\[
\tilde{H}_a = -2k'^{ij}_{a;i} P^{ij} + K'^{ij}_{ij;a} P^{ij} \approx 0 \quad \text{(2.16a)}
\]

Note, however that the covariant derivative still has the metric \(h^{ij}\) (in the connection) that must be replaced by \(p^{ij}\). After some algebra we obtain,

\[
\tilde{H}_a = -2k'^{ij}_{a;i} P^{ij} - 2k'^{ij}_{a;i} P^{ij} + K'^{ij}_{ij;a} P^{ij} \approx 0 \quad \text{(2.16b)}
\]

To understand the physical meaning of this constraint, we calculate its Dirac bracket with \(K'^{ij}_{ij}\) and with \(P^{ij}\),

\[
\{K'^{kl}_{kl}(x), \int d^{d-1} y \xi^a(y) \tilde{H}_a(y)\}^* = \xi^a_{;i} K'^{ij}_{ia} + \xi^a_{,k} K'^{ij}_{ka} + \xi^a K'^{ij}_{kl,a}
\]
Thus, we can see that they transform respectively as a tensor and as a tensor density of weight one under coordinate transformations on the hypersurface. The meaning of the constraint is then, essentially, the same in both representations, showing also that $K'_{ij}$ is indeed the relevant canonical variable to be considered in the quantization.

The constraint (2.13a) is, in terms of $K'_{ij}$ and $P^{ij}$,

$$
H_0 = \left( \frac{P}{4} \right) (d-3)^{-1} \frac{R_{ij}P^{ij}}{2} + \left[ \frac{(d - 1)}{2(d - 2)} K'_{mn} K'_{ij} - K'_{mj} K'_{in} - K'_{ni} K'_{mj} \right] p^{mn} p^{ij} \approx 0 \tag{2.17a}
$$

where,

$$
\left( \frac{P}{4} \right) (d-3)^{-1} \frac{R_{ij}P^{ij}}{2} = (2^{1-d} P) (d-3)^{-1} \left[ -P^{ij}_{,ij} - \frac{1}{4} P_{ij} P^{bd} P^{ij}_{,bd} + \frac{1}{2} P_{ij} P^{ab} P^{ij}_{,a} + \frac{1}{4(d-3)} (-4 P_{ij} P^{ab} P^{ij}_{,b} + (d - 7) P_{ij} P^{kl} P^{ij}_{,kl}) + (d - 7) P^{kl} P^{ij}_{,k} + P_{ij} P^{ab} P^{ij}_{,ab} \right] \tag{2.17b}
$$

This concludes the construction of the classical theory in first order form. We checked that the imposition of the new constraints that appear in the first order formalism implies in particular expressions for Lagrange multipliers that are in agreement with what one obtains from Hamilton's equations of motion. We reduced some of the second class constraints to first class, and showed how the introduction of the Dirac brackets transforms the remaining second class constraints into strong identities between the canonical variables allowing two different representations of the first class constraints; the first case considered ($h^{ij}$ and $\pi'_{ij}$ ) gives rise to the super-momentum and super-Hamiltonian constraints familiar from the second order formalism. The second choice ($K'_{ij}$ and $P^{ij}$ ) gives rise to the generator.
of coordinate transformations on the hypersurface for the relevant canonical variables and to a modified super-Hamiltonian constraint whose meaning will be further clarified in the next section.

3. Canonical Quantization

We are now ready to quantize the theory following the usual steps. Note that we have a choice between two pairs of canonical variables due to the second class constraints. We start with the pair \((\hat{h}^{ij}, \pi'_{ij})\): First the canonical variables are turned into operators with the Dirac brackets becoming the usual commutation relations,

\[
[h^{ij}(x), \pi_{kl}(y)] = i\delta_{kl}^{ij}\delta(x - y) .
\]

These operators are substituted into the super-momentum (eq.(2.15a)) and into the super-Hamiltonian (eq.(2.15b)) constraints that are then turned into operators. The constraints are applied into the states \(\Psi\) selecting those that are physically permissible, (from now on we suppress the carets on quantum operators)

\[
\hat{H}_0 \Psi(h) = h^{ij}\left(\frac{\delta \Psi}{\delta h_{ij}}\right)_j = 0
\]

(3.1)

\[
\hat{H}_0 \Psi(h) = \left(\frac{\delta^2 \Psi}{\delta h^{ij}\delta h^{kl}} + h^{1/2}\tilde{R}\right)\Psi(h) = 0 ,
\]

(3.2)

where we have chosen the "\(h^{ij}\)" representation with \(\pi'_{ij} = -i\frac{\delta}{\delta h^{ij}}\) and \(\Psi = \Psi(h^{ij})\). Also,

\[
G^{ijkl} = \frac{1}{2}h^{-1/2}[h^{ik}h^{jl} + h^{il}h^{jk} - \frac{2}{(d-2)}h^{ij}h^{kl}]
\]

(3.3)

is the metric of superspace, the space of all positive definite \(d-1\) -metrics.
We have not solved the factor ordering problem. Following the standard procedure [1], we have chosen to put the metric terms on the left of the momenta in the super-momentum constraint, eq.(3.1), since with this choice its interpretation is more transparent: The wave functional $\Psi(h)$ is independent of the particular choice of representation for the metric components $h^{ij}(x^k)$ in some system of coordinates $x^i$. The argument of the wave functional then belongs to the space of all metrics identified by a $d - 1$ diffeomorphism [7].

The super-Hamiltonian constraint, eq.(3.2), is the “Wheeler-DeWitt" equation in its usual representation. We are also leaving aside the difficult problem of constructing a Hilbert space from the space of solutions of (3.2). We will come back to this question later on.

Now we repeat the same steps for the other pair of coordinates, $(K^i_{ij}, P^i_{ij})$. Choosing the “$K'$" representation, we have that, $P^i_{ij} = -i\frac{\delta}{\delta K^i_{ij}}$ and $\Psi = \Psi(K^i_{ij})$. The super-momentum and super-Hamiltonian constraints are, respectively,

$$\bar{H}_a \Psi = -2K_{aij}^i \frac{\delta \Psi}{\delta K^i_{ij}} - 2K^i_{ij} \left( \frac{\delta \Psi}{\delta K^i_{ij}} \right) + K^i_{ij,a} \frac{\delta \Psi}{\delta K^i_{ij}} = 0$$

(3.4)

$$\bar{H}_0 \Psi = \left[ \left( K^i_{mj}^i K^i_{ni} + K^i_{mi} K^i_{nj} - \frac{(d - 1)}{2(d - 2)} K^i_{ij} K^i_{mn} \right) \frac{\delta^2}{\delta K^i_{ij} \delta K^i_{mn}} + F(\frac{\delta}{\delta K^i_{ij}}) \right] \Psi = 0$$

(3.5)

where $F(\frac{\delta}{\delta K^i_{ij}})$ is obtained using eq. (2.17b) with $P^i_{ij} = -i\frac{\delta}{\delta K^i_{ij}}$ and $P_{ij} = -i\frac{\delta}{\delta K^i_{ij}}$.

If we perform an infinitesimal coordinate transformation, $\bar{x}^i = x^i + \xi^i(x^k)$ and note that $K^i_{ij}$ transforms as,

$$\delta K^i_{ij} = \xi^a_i K^i_{ja} + \xi^a_i K^i_{ia} + \xi^a_i K^i_{ij,a} ,$$

it is easy to show that the super-momentum constraint has precisely the same meaning as in the other representation.
The constraint (3.5) is a new representation for the Wheeler-DeWitt equation defined now in the functional space of $K'_{ij}$. Note that this representation can only be obtained by using the first-order formalism and is not simply a Fourier transform of the original equation. Although we expect the physics to be the same in both representations, this equation gives the probability amplitude for having a hypersurface with some $K'$, thus providing information on the dynamics of the embedding of the hypersurface in spacetime. We hope to explore the consequences of this equation further [9].

As another illustration of the first-order formalism, we briefly show how other representations of the Wheeler-DeWitt equation can be generated by playing with total derivatives in the original action, eq.(2.2). First, consider integrating by parts the second term in (2.2); in this way, the time derivative of the metric appears only in its determinant and the action becomes,

$$I[h^{ij}, K_{ij}, N^i, N^j] = \int d^{d-1}x dt (-h^{1/2} h^{ij} \dot{K}_{ij} + K \dot{h}^{1/2} - \lambda_0)$$

(3.6)

If we follow the previous steps for the construction of the classical theory, we soon find that $h^{ij}$ is not the appropriate canonical variable but $h^{1/2}$. We then write $h^{ij} = (h^{1/2})^a \tilde{h}^{ij}$, where $a = -2/(d - 1)$ and $\text{det} \tilde{h}^{ij} = 1$. The conjugate momentum to $h^{1/2}$ is, $\pi = K = (h^{1/2})^a \tilde{h}^{mn} K_{mn}$ and we must add the constraint $\varepsilon (\text{det} \tilde{h}^{ij} - 1)$ to the Lagrangian, where $\varepsilon$ is a Lagrange multiplier. We then construct the Dirac brackets and find that the correct momentum conjugate to $h^{1/2}$ is $\pi' = 2(d - 2)/(d - 1)K$. In the quantum version, $\pi'$ is identified with $-i \frac{\delta}{\delta h^{1/2}}$. Thus, in the super-Hamiltonian constraint the "intrinsic time" $(h^{1/2})$ appears naturally. Likewise, writing $K_{ij}$ in terms of its traceless and trace parts (treating them as independent variables) and using the second class constraints, we could
have obtained the Fourier transform of $\tilde{h}^{ij}$ in the "extrinsic time" ($K$) approach to the Wheeler-DeWitt equation [9]. If we continue to explore the possibilities of the first order action, we can find various different representations of the Wheeler-DeWitt equation, some of them not yet known in the literature. We stress that this is only possible within the first order formalism, since in the second order formalism the action is quadratic in the velocities not allowing for partial integrations. Also, in the second order formalism we cannot use the traceless and trace parts of $K_{ij}$ as canonical variables to reproduce the above results.

4. Conclusion

We have constructed a first order formalism for Einstein gravity within the ADM formulation. After classifying all the constraints as second class, we showed how some of them can be reduced to first class by using the arbitrariness in the lapse function and shift vector and the fact that the total Hamiltonian is a first class constraint by construction. By introducing Dirac brackets, we reduced the remaining second class constraints to identities between pairs of canonical variables that allow us to choose between two possible representations, the $h^{ij}$ and the $K'_{ij}$ representations. We then quantized the theory using the canonical method and found that the first representation reproduces the well known super-momentum and super-Hamiltonian constraints obtained in the second order formalism whereas the second choice gives rise to a new representation of the Wheeler-DeWitt equation, defined in the functional space of a modified extrinsic curvature $K'_{ij}$.

We plan to try to solve it in the mini-superspace in the hope that using the connection between $K$ and the expansion of the Universe we will obtain some insight into the arrow
of time problem.

We have also showed how the first order formalism can generate many representations of the Wheeler-DeWitt equation by manipulation of total derivatives in the action and identification of the relevant canonical variables. As an example, we indicated how to obtain the extrinsic and intrinsic time representations. We hope that by finding different representations of the Wheeler-DeWitt equation, more will be learned about the physics behind it.

As mentioned in the introduction, the first order formalism can play a very important role in the quantization of theories with higher-order terms in the curvature. In particular, we note the similarity between Einstein gravity and the EGB theory in the sense that both have $\dot{K}_{ij}$ terms as surface terms contrary to other curvature squared actions. The Wheeler-DeWitt type equation in the EGB theory can be written, after a functional Fourier transform between the metric and its conjugate momentum, as a functional equation for $\Psi(\pi)$, as in the case for Einstein gravity. The difference between the two theories arises because, while in the Einstein gravity case the $\pi_{ij}$ is related linearly with $K_{ij}$, in the EGB case the momentum is given by a complicated expression involving the extrinsic and intrinsic curvatures of the hypersurface. Thus, the advantage of going to the first order formalism is clear in the latter case: The $(K'_{ij}, P^{ij})$ representation will indeed allow us to obtain an equation for the wave-function which will be a functional only of the extrinsic curvature, providing information about the expansion of the Universe.

Finally, we would like to make some remarks on the Hilbert space problem of quantum gravity. Going back to the intrinsic time representation, we can, after some algebra, write
the super-Hamiltonian constraint as (note that we are not using the second class constraints yet)

\[
\left[ \hbar^{1/2}(\mathcal{K}^2 - K_{ij}K^{ij}) + 2(\hbar^{1/2})^{2/(d-1)}(K_{ij} - \frac{h_{ij}K}{d-1})\tilde{\pi}_{ij} + \right.
- \frac{2(d-2)}{d-1}\hbar^{1/2}K\pi' + (R_{ij} + KK_{ij} - 2K_{ip}K_{pj})P^{ij} - P^{ij}_{;ij}\right] \Psi = 0 \tag{4.1}
\]

where we must make the substitution \( K_{ij}' = K_{ij} + \frac{1}{d-3} h_{ij}K \), in order to write

\[
\pi' = -i \frac{\delta}{\hbar^{1/2}} ; \quad \tilde{\pi}_{ij} = -i \frac{\delta}{\hbar^{1/2}} ; \quad P^{ij} = -i \frac{\delta}{\delta K_{ij}}
\]

Also, \( \Psi = \Psi(h^{1/2}, \tilde{h}_{ij}, K_{ij}') \). The second class constraints are \( \pi = K \); \( \tilde{\pi}_{ij} = 0 \); \( P^{ij} = -\hbar^{1/2}h_{ij} \).

We can see that \( \pi' \) plays the role of a time derivative on superspace, thus making the above equation a Schrödinger-like equation. It remains to be seen if it is possible to construct a Hilbert space based on the solutions of this equation before imposing the second class constraints.

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