Hamiltonian reduction of spin-2 theory and solvable cosmologies

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Abstract
The Hamiltonian reduction of the massless spin-2 field theory is carried out following the Faddeev–Jackiw approach. The reduced Hamiltonian contains only the traceless-transverse fields, but not all of the non-propagating components can be determined by the constraints of the theory. The reason for this is found in the fact that the Hamiltonian is not gauge invariant. Consequences and implications for general relativity are discussed and illustrated on the example of Robertson–Walker cosmologies with a scalar field. Also, it is shown that for these explicitly solvable models, the reduced form of the dynamics uniquely determines the operator ordering that has to be adopted in the Wheeler–DeWitt equation in order to maintain consistency.

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1. Introduction

It is generally believed that the free, massless spin-2 field is entirely determined, in the Hamiltonian formulation, by the dynamical equations for the propagating (radiative) modes and by the constraints of the theory. Although this is supported by a naive counting argument (two propagating modes, four constraints and four undetermined gauge variables), we argue in this paper that this assumption is actually mistaken. The reason can be recognized in different ways, for instance in the fact that the Hamiltonian is not gauge invariant off the constraint surface. A similar situation holds in general relativity. Although the analysis is difficult to carry out in the full theory, it is not hard to illustrate the corresponding issues by means of simple examples for which the Hamiltonian reduction can be carried out explicitly. A consequence of this particular feature is the fact that there exist spacetimes that are not classical, but are nevertheless free of dynamical quantum gravitational fields, i.e. in the linear approximation, of gravitons. More precisely, there exist field configurations for which there are no dynamical gravitational fields (i.e. field components that are directly turned into quantum operators via the correspondence principle), but nevertheless the same configurations may contain metric components that are to be described by operators in the quantum theories, in
contrast to the constrained fields, which remain classical. This comes about because, as we will show, the dynamical fields and the constrained fields alone do not describe completely the physical situation. Instead, it is necessary to determine in addition some of the remaining components (usually referred to as Lagrange multipliers). The equations which determine these multipliers, however, contain some of the dynamical fields (gravitational or matter), and are thus, in the quantum theory, to be interpreted as operator relations. This situation is quite different from conventional gauge theories, where the gauge-invariant (and hence physical) quantities can all be determined without the knowledge of the multipliers.

As a by-product of our analysis, we show that the explicitly reduced theory dictates the operator ordering that has to be adopted in the Wheeler–DeWitt equation in order to find results that are consistent with those from the reduced theory.

The paper is organized as follows. In the following section, we deal with the special relativistic spin-2 theory. In section 3, arguments are presented that the situation can be expected to be similar in the framework of general relativity. In the remaining sections, this is explicitly demonstrated on the example of Robertson–Walker cosmologies with scalar field (section 4), where we carry out the Hamiltonian reduction (section 5) and compare with the Wheeler–DeWitt approach (section 6), as well as with the results obtained from the fixation of the time coordinate (section 7). Finally, in section 8, we perform a change of variables such that the resulting theory is trivially reducible and the corresponding Wheeler–DeWitt equation is free of operator ordering problems.

2. Spin-2 theory

We start from the first-order Lagrangian (see, e.g., [1] for its derivation from the second-order Fierz–Pauli Lagrangian)

\[ L = \pi_{\mu\nu} \dot{h}_{\mu\nu} - H(\pi_{\mu\nu}, h_{\mu\nu}) + h_{0\mu}(2\pi_{\mu\nu},,\nu) + h_{00}(\frac{1}{2}h_{\mu\nu},,\mu ,\nu + \frac{1}{2}h_{,\mu},\mu), \]  
(1)

where our signature convention is \( \eta_{\mu\nu} = -\delta_{\mu\nu} \) \( \mu, \nu = 1, 2, 3 \), \( h = h_{\mu\nu} \). We will further use the notations \( \Delta A = \dot{A} \partial_{\mu}A = A^{,\mu}_{,\mu}, \) and \( \Box A = \dddot{A} + \Delta A \), where the dot denotes the time derivative. The Hamiltonian has the form

\[ H = \pi^{\mu\nu} \pi_{\mu\nu} - \frac{1}{2} \pi^2 + \frac{1}{2} h_{,\mu} h^{,\mu} - \frac{1}{4} h^{\nu\lambda},,\mu h_{\nu\lambda},,\mu + \frac{1}{2} h^{\nu\lambda},,\mu h_{,\nu\lambda},,\nu - \frac{1}{2} h^{\mu\nu},,\mu h_{,\mu},,\nu. \]  
(2)

In the first three sections of this paper, integration over space is always understood and surface terms will be discarded whenever necessary. Note that we call Hamiltonian only the above expression, without the constraints coupled to it. The absence of \( h_{0\mu} \) and \( h_{00} \) in the kinetic term of \( L \) leads to the constraints

\[ 2\pi^{\mu\nu},,\mu = 0, \quad -\frac{1}{2} h^{\mu\nu},,\mu + \frac{1}{2} \Delta h = 0. \]  
(3)

The Lagrangian (1) is easily shown to be invariant under the following gauge transformations:

\[ \delta h_{\mu\nu} = \xi_{\mu},,\nu + \tilde{\xi}_{\nu},,\mu, \]  
(4)

\[ \delta \pi_{\mu\nu} = -\varepsilon,\mu,;\nu + \eta_{\mu\nu} \Delta \varepsilon, \]  
(5)

\[ \delta h_{0\mu} = \dot{\xi}_{\mu} + \varepsilon,\mu, \quad \delta h_{00} = 2\dot{\varepsilon}. \]  
(6)

This is a consequence of the invariance of the second-order Lagrangian under \( \delta h_{ik} = \xi_{i},,k + \xi_{k},,i, \) \( i, k = 0, 1, 2, 3 \), with \( \xi_0 = \varepsilon \). It is needless to say that (4) and (5) are induced by the constraints (3). The reduction to the dynamical degrees of freedom consists of solving the constraints explicitly and bringing the Hamiltonian into a form that contains only the physical fields. This has been done in [2] starting from a slightly different (but equivalent) Lagrangian,
and also in [1], where we have reduced the spin-2 Hamiltonian following along the lines of Faddeev and Jackiw [3]. The essential step is to express the fields \( h_{\mu\nu} \) and the momenta \( \pi_{\mu\nu} \) in terms of the traceless-transverse (TT) parts \( ^{TT}h_{\mu\nu} \) and \( ^{TT}\pi_{\mu\nu} \) respectively, and to recognize that, on the constraint surface, the remaining fields (longitudinal, trace) cancel out both in the kinetic term and in the Hamiltonian. In other words, on the constraint surface, we have

\[
L_R = ^{TT}\pi_{\mu\nu} ^{TT}h^{\mu\nu} - H_R(^{TT}\pi_{\mu\nu}, ^{TT}h_{\mu\nu}),
\]

with

\[
H_R = ^{TT}\pi_{\mu\nu}^{TT}h^{\mu\nu} - \frac{1}{2} ^{TT}h^{\mu\nu, \lambda} ^{TT}h_{\mu\nu, \lambda}.
\]

The index is attached to \( H_R \) (and \( L_R \)) to remind that this form of \( H \) (and \( L \)) holds only if the constraints are satisfied. The equal time Poisson brackets can be read from (7) as

\[
[H, ^{TT}\pi_{\mu\nu}] = -^{TT}\pi_{\mu\nu}, \quad [H, ^{TT}h_{\mu\nu}] = -^{TT}h^{\mu\nu},
\]

which lead to the expected wave equation of the spin-2 particle, \( \Box ^{TT}h^{\mu\nu} = 0 \). As expected, the reduction straightforwardly leads to the identification of the propagating field modes, and the transition to the quantum theory is now possible. However, it is obvious that the dynamical equation (9), together with the constraints (3), does not determine the system completely. In other words, (9) and (3) are not equivalent to the set of field equations that can be derived from the Lagrangian (1) (or, alternatively, directly from the second-order Fierz–Pauli Lagrangian, see [1]). In fact, variation of \( L \) with respect to \( h_{\mu\nu} \) and \( \pi_{\mu\nu} \) leads to field equations whose traces respectively are

\[
\ddot{h} + \pi - 2h^{\mu\nu, \mu} = 0, \quad \ddot{\pi} + \frac{1}{2} \Delta h - \frac{1}{2} h^{\mu\nu, \mu, \nu} + \Delta h_{00} = 0,
\]

leading to the configuration-space equation

\[
\ddot{h} + h_{00} - 2h^{\mu\nu, \mu} = 0,
\]

where we have already used one of the constraints. These equations, which are gauge invariant, cannot be obtained merely from the constraints (3) and the dynamical equation (9), as is easy to see (consider, e.g., the configuration \( \pi_{\mu\nu} = h_{\mu\nu} = h_{00} = 0, h_{00} = \exp(-r) \), which solves (3) and (9), but is not a solution to (10) or (11)). It is not hard to argue that there are no other independent equations one obtains from (1) that are not contained in the constraints and in the dynamical equations, see [1].

We conclude that the spin-2 field is not entirely characterized by the dynamical and constraint equations alone, in sheer contrast to conventional gauge theories, and we will now analyze both the reasons and the consequences of this observation. It is known that the Hamiltonian reduction sometimes leads to a loss of information. For instance, it has been demonstrated in [4] that this can happen in systems with ineffective constraints. Somewhat more close to our case are systems with the so-called reducible constraints, i.e. constraints that are not independent, see [5, 6]. The classical example is that of constraints of the form \( p^{\mu\nu, \mu} = 0 \), with antisymmetric \( p^{\mu\nu} \). These constraints are interrelated via \( p^{\mu\nu, \mu, \nu} = 0 \) and therefore cannot generate independent gauge transformations. Here, we have a slightly different situation, namely the constraints \( \frac{1}{2} G^{00} = \frac{1}{2} (\Delta h - h^{\mu\nu, \mu, \nu}) \) and \( G^{0\mu} = 2\pi^{\mu\nu} \), satisfy the relation \( G^{00} + G^{0\mu} = 0 \). This is a result of the Bianchi identities of the linear spin-2 theory. (Recall that \( G^{00} = 0 \) and \( G^{0\mu} = 0 \) are nothing but the field equations corresponding to \( h_{00} \) and \( h_{0\mu} \) respectively, i.e. they are equal to the corresponding components of the linearized Einstein tensor, expressed in phase-space variables. Note, however, the factor 2 that results
because $G^{ik}$ is defined upon variation with respect to $h_{ik}$, whose components are not the same as those obtained upon direct variation with respect to $h_{\mu\nu}$, $h_{00}$, and $h_{0\mu}$, since in products like $a_{ik}a^{ik}$ the mixed components $a_{0\mu}$ occur twice.) However, in contrast to the case of reducible constraints, the interrelation of the constraints manifests itself only on-shell, since we have to use the explicit expressions for $\pi_{\mu\nu}$ in terms of $h_{\mu\nu}$. Nevertheless, we retain the fact that, strictly speaking, the constraints are not independent.

A more obvious reason why the reduction must lead to the loss of a field equation can be seen in the following. As is easily shown, the solutions to the second constraint in (3) can be written in the form $h_{\mu\nu} = TT_{h_{\mu\nu}} + f_{\mu,\nu} + f_{\nu,\mu}$ (see [1] or [2] for the explicit expression of $f$), meaning that $h_{\mu\nu}$ is TT, up to a gauge transformation. If we now choose the particular gauge $h_{\mu\nu} = TT_{h_{\mu\nu}}$, and further impose $\pi = 0$, which can be achieved with (5) with a suitable choice of $\epsilon$, then the first of equation (10) reduces to $h_{\mu\nu}^{00} = 0$ and the second to $\Delta h_{00} = 0$. But these equations are now in the form of constraints, i.e. they do not depend on velocities. Thus, depending on the gauge one adopts, these equations appear either in the form of constraints or in the form of dynamical equations. Therefore, they cannot be obtained as dynamical equations of the form $[H, A] = -A$, for some physical (gauge invariant) variable $A$, nor can they arise as true constraints, at least not as long as we do not explicitly fix the gauge. Obviously, the Hamiltonian reduction process, which is based on solving the constraints and introducing Poisson brackets for the physical variables only, has no place for such an intermediate case.

The mathematical reason for the failure of the reduction process is simply the fact that the Hamiltonian (2) is not gauge invariant off the constraint surface, in contrast to conventional gauge theories. Let us illustrate this on the example of electrodynamics, where we have

$$L = \pi^\mu A_\mu - H + A_0 \pi^{\mu,\mu},$$

(12)

with

$$H = -\frac{1}{2} \pi_{\mu\nu} \pi^{\mu\nu} + \frac{1}{2} F_{\mu\nu} F^{\mu\nu},$$

(13)

and we find $\delta \left( \pi^\mu A_\mu + A_0 \pi^{\mu,\mu} \right) = 0$, as well as $\delta H = 0$ under $\delta \pi_{\mu\nu} = 0$, $\delta A_\mu = \varepsilon_{,\mu}$, $\delta A_0 = \dot{\varepsilon}$. This means that the gauge-dependent parts of $A_\mu$ (the longitudinal modes) are not contained in $H$, independently of whether we are on or off the constraint surface. The reduced Hamiltonian is given by

$$H_R = -\frac{1}{2} \pi_{\mu\nu} T_{\mu\nu} + \frac{1}{2} A_{\mu,\nu} T^{\mu\nu},$$

(14)

where $T_{\mu\nu}$ is the transverse field. Note that for the magnetic field, we have $F_{\mu\nu} = A_{\nu,\mu} - A_{\mu,\nu} = T_{A_{\nu,\mu}}$, while the electric field is given by $\pi^\mu$. Both are obviously gauge invariant and, moreover, they constitute the only gauge-invariant quantities of the theory. (This can easily be generalized to the case where charged matter fields are present, see, e.g., [3].) The point is that both the electric and the magnetic fields are completely determined by the dynamical variables $T_{\pi^\mu}$ and $T_{A_{\mu}}$ and the constraint alone, since the only non-dynamical field occurring in these fields is the longitudinal component of $\pi^\mu$, which is fixed by the constraint $\pi^{\mu,\mu} = 0$.

On the other hand, in the spin-2 theory, we have a different situation. First, we note that for the transformations induced by $\xi_{\mu\nu}$ according to (4)–(6) we again have $\delta \xi H = 0$ as well as $\delta \xi \left( \pi^{\mu\nu} h_{\mu\nu} + h_{00} \frac{1}{2} G^{00} + h_{0\mu} G^{0\mu} \right) = 0$, where we again use the symbols $\frac{1}{2} G^{0\mu}, G^{0\mu}$ for expressions (3). This is just as in electrodynamics.

Quite in contrast, however, for the transformations induced by $\varepsilon$, although the total Lagrangian is invariant, we find

$$\delta \varepsilon H = 2 \pi^{\mu\nu,\nu} \varepsilon_{,\mu},$$

(15)
which shows that \( H \) is not invariant off the constraint surface. Obviously, this variation is compensated by the variation of other terms in \( L \). Indeed, we find \( \delta_v(H + h_{00}, 2\pi_{\mu\nu}) = 0 \).

Thus, the Hamiltonian \( H \), in contrast to its electromagnetic counterpart, is not independent of the gauge variables. As a result of this, although the total Lagrangian is (by construction) gauge invariant, we simply cannot discard the gauge variables (as can be done with the longitudinal parts of \( A_\mu \)) and simultaneously treat \( h_{00} \) and \( h_{0\mu} \) as arbitrary Lagrange multipliers (as can be done with \( A_\mu \)). We can do either one or the other, but not both, in contrast to what seems to be the belief in [2]. On the level of the field equations, this is clearly demonstrated by the fact that these variables are interrelated by equation (10) or (11). If we discard the gauge variables and directly replace \( h_{\mu\nu} \) and \( \pi_{\mu\nu} \) by \( ^{TT}h_{\mu\nu} \) and \( ^{TT}\pi_{\mu\nu} \) respectively, then \( h_{00} \) and (or) \( h_{0\mu} \) cannot be arbitrary, and are determined by equation (11). Alternatively, if we fix the Lagrange multipliers to, e.g., \( h_{00} = h_{0\mu} = 0 \), then (11), which is not identically satisfied on the constraint surface, determines the trace of \( h_{\mu\nu} \). We will see these features more explicitly in the framework of general relativity later on.

Since the variation of the Hamiltonian leads to a term proportional to the constraint, see (15), the above-described interrelation gets lost once we solve the constraints. This is the reason why the reduction process leads to a loss of information. It is important to recall once again that this information is of physical relevance and cannot be discarded, since equation (10) is gauge invariant.

From the above considerations, one can conclude that there exists no Coulomb gauge for the spin-2 field, i.e. a gauge where all equations but the dynamical (TT) are free of time derivatives, i.e. of the form of a Gauss-type law. Indeed, as we have outlined above, it is possible, e.g., to choose \( h_{\mu\nu} = ^{TT}h_{\mu\nu} \) and \( h^{\mu\nu,\mu} = 0 \), such that field equations reduce to \( \Delta h_{00} = \Delta h_{0\mu} = 0 \) (with solutions \( h_{00} = h_{0\mu} = 0 \) and \( \Box ^{TT}h_{\mu\nu} = 0 \) respectively. But this is not a Coulomb gauge. It is the analog of the radiation gauge \( A_0 = 0 \) and \( A_\mu = ^{TT}A_\mu \) in electrodynamics, which is, strictly speaking, not a gauge, but rather a combination of the transverse gauge and the solution of Gauss’ law \( \Delta A_0 = 0 \). The existence of this radiation gauge has been known at least since the works on gravitational waves by Einstein and Rosen, and is demonstrated in any textbook on general relativity. For the Coulomb gauge, we need something more. The difference to the electromagnetic case lies in the fact that in Maxwell’s theory, the transverse gauge can be imposed on \( A_\mu \) independent of whether or not \( A_\mu \) is a solution to the constraint (in fact, in phase space, the constraint equation \( F^{\mu\nu}_{\rightarrow\mu} = 0 \) has the form \( \pi^{\mu}_\mu = 0 \) and does not even depend on \( A_\mu \)). In the spin-2 case, on the other hand, the TT gauge is only possible if \( h_{\mu\nu} \) is a solution to the constraint \( h^{\mu\nu,\mu} = \Delta h = 0 \). In the general case [2], we have a decomposition \( h_{\mu\nu} = ^{TT}h_{\mu\nu} + ^{TT}h_{\mu\nu} + f_{\mu\nu} + f_{\mu\nu} \), where the transverse part \( ^{TT}h_{\mu\nu} \) cannot be gauged away. Only on the constraint surface, we have \( ^{TT}h_{\mu\nu} = 0 \). Why is this of importance? Well, suppose we couple the field to some matter field. Then the constraint changes, and so does the solution to the constraint. For instance, if we see in the spin-2 theory the linearized approximation of general relativity, then the constraint would take the form \( G_{00} - \rho = 0 \), where \( \rho = T_{00} \) is a component of the stress–energy tensor of the matter fields. The solution to this constraint can be written in the form \( h_{\mu\nu} = ^{TT}h_{\mu\nu} + f_{\mu\nu} + f_{\mu\nu} + \eta_{\mu\nu} \rho / \Delta \), see [1], and this is not gauge equivalent to \( ^{TT}h_{\mu\nu} \) anymore. Thus, we cannot reduce \( h_{\mu\nu} \) to its propagating components only. As a result, there is no Coulomb gauge, because even if we solve the four constraints (3), which can be viewed as the analog to Gauss’ law, there will remain, apart from the dynamical equations, one more equation in the form of (11), eventually with sources, where \( h \) cannot be eliminated.

Summarizing, in contrast to the situation in the Maxwell theory, the TT-gauge condition can only be imposed on the constraint surface. In other words, the TT gauge does not exist in the strict sense. There are only particular solutions (namely, the radiative solutions) that can be
brought into that form. For this reason, in textbooks on general relativity, an explicit reference to wave solutions has to be made in order to demonstrate the TT nature of gravitational waves, quite in contrast to electrodynamics, where the transversality condition can be trivially imposed right from the outset.

A potential danger of these specific features of the spin-2 theories lies in the following. Suppose that, for some reason, we work with a reduced number of degrees of freedom, i.e. we make some ansatz for $h_{\mu\nu}$, $\pi_{\mu\nu}$, $h_{0\mu}$ and $h_{00}$. Further suppose that the number of independent functions we describe our fields with cannot be reduced any further by a gauge transformation. If we then solve the constraints, we still cannot conclude that the remaining set of independent functions (that are not fixed by the constraints) must correspond to the physical variables of the theory, as would be the case in a conventional gauge theory. In particular, we simply cannot assume that the unconstrained variables are subject to second quantization, because even when the gauge is fixed and the constraints are solved, there still remains one degree of freedom in the theory that is not a physical (propagating) field.

If we assume for the moment that we have a similar situation in general relativity (as we will see in the following sections), then the above remark turns out to be of particular relevance. For instance, if we start from the outset with, e.g., a cosmological function and a scalar (matter) field only, then it is not at all obvious that these functions are indeed part of the dynamical fields and that, consequently, we should replace them with quantum operators satisfying canonical commutation relations. In fact, the cosmological function (appearing as a conformal factor in front of the three-dimensional metric) is actually, in the weak field limit, related to the trace $h$ of the metric perturbation $g_{ik} = \eta_{ik} + h_{ik}$, which, however, appears in equation (11) rather than in the dynamical equation (9). Indeed, it turns out that the cosmological function is not a dynamical variable.

3. General relativity

The important question is to what extent our considerations can be generalized to the self-interacting, generally covariant theory, to general relativity. For the Hamiltonian formulation of general relativity, we refer to [7–10]. The explicit reduction of the theory is a highly difficult task, due to the nonlinearity of the constraints. In the focus of the analysis is the identification of the physical variables. There are again two dynamical degrees of freedom and we will denote the corresponding pair of canonical variables with $TT \pi_{\mu\nu}$ and $TT g_{\mu\nu}$, see [8, 9]. In fact, it has been argued in [9] that the similarity to the linear theory is actually quite strong, in particular with respect to the choice of the canonical variables, since the nonlinearity of the theory expresses itself mainly in the constraints, and not in the kinematical sector of the Lagrangian. The first-order Lagrangian is of the form [10]

$$L = \pi^{\mu\nu} g_{\mu\nu} - N \mathcal{H} - N_{\mu} \mathcal{H}^{\mu},$$

where the constraints $\mathcal{H} = \mathcal{H}^{\mu} = 0$ are equivalent to four of Einstein’s equations, $G^{00} = G^{0\mu} = 0$, expressed in terms of $g_{\mu\nu}$ and $\pi^{\mu\nu}$ (see [10] for the explicit expressions). The Hamiltonian itself is zero (compare with (1)) and, thus, the equations for the physical fields are simply $TT g_{\mu\nu} = TT \pi^{\mu\nu} = 0$. Since we have not solved explicitly the constraints, we do not know exactly which parts of the fields correspond to the physical (TT) parts, but we know that they are contained in $\pi^{\mu\nu}$ and $g_{\mu\nu}$ (and not in $N$, $N_{\mu}$). Note that the non-TT parts of $\pi^{\mu\nu}$ and $g_{\mu\nu}$ do not necessarily have a vanishing time derivative, because, since these variables appear in the constraints, for the derivation of the corresponding equations of motion, the full Hamiltonian $H + N \mathcal{H} + N_{\mu} \mathcal{H}^{\mu}$ (with $H = 0$) has to be used.
If one assumes that, as in conventional gauge theories, the configuration is determined by the constraints and by the dynamical equations alone, then, since the latter are trivial, one comes to the conclusion that the complete information must be contained in the constraints alone. On the other hand, the linear theory shows that this is not necessarily the case. There might well be an additional equation that is neither dynamical nor a constraint. Evidence that this is indeed the case comes from several directions. For one, there is of course the fact that there is a direct link between general relativity and its linear counterpart. The perturbation theory should to first-order reproduce the results that we find for the linear theory. Further, as a result of the Bianchi identity $G^{ik}_{\,;k} = 0$, we see that the constraints are again on-shell related. One can also try to construct a metric such that the Einstein field equations contain second time derivatives of three independent functions, demonstrating in that way the fact that the corresponding set of first-order equations contains at least three pairs of equations that are not constraints, which is one more than there are physical degrees of freedom (see [1] for such an attempt). It turns out to be easier to demonstrate directly that the set of constraints and dynamical equations is underdetermined with an explicit example. For instance, if we take $g_{\mu\nu} = \eta_{\mu\nu}, \pi^{\mu\nu} = N_\mu = 0$ and $N^2 = \exp(-r)$, then both the constraints $\mathcal{H} = 0$ and $\mathcal{H}_\mu = 0$, as well as the dynamical equations, are trivially satisfied (the latter because we have $g_{\mu\nu} = \pi^{\mu\nu} = 0$ and, thus, the same holds in particular for the TT parts, while for the former, consider the explicit form of the constraints as given in [10]). Nevertheless, the above configuration is not a solution to the complete set of the Einstein field equations in a Hamiltonian form. This shows that there must be an extra equation apart from the constraints and the TT equations. Indeed, one can directly verify that the equation $\mathcal{R} = 0$, with $\mathcal{R}$ as the four-dimensional curvature scalar, expressed in terms of $g_{\mu\nu}, \pi^{\mu\nu}, N$ and $N_\mu$, is not fulfilled for the above configuration. Although this equation contains gauge fields (non-TT parts), as well as $N$ and $N_\mu$, it cannot be argued that the equation is physically irrelevant. These fields cannot be considered to be completely arbitrary, but rather transform in a well-defined way, such that altogether, the equation transforms into itself (after all, $\mathcal{R}$ is a scalar!).

One can also argue as follows. If one again considers the trace of the Einstein field equations, $\mathcal{R} = 0$ (the explicit expression for $\mathcal{R}$ can be found in [10]), then one recognizes that the only time derivative is contained in a term of the form $(g_{\mu\nu}\pi^{\mu\nu})$, or simply $\dot{\pi}$. Therefore, if we choose the gauge $N = 1, N_\mu = 0$, then the equation $\mathcal{R} = 0$ contains velocities, namely $\dot{\pi}$. Choosing instead the gauge $\pi = 0$ (e.g., together with $(\sqrt{g} g^{\mu\nu} g_{\mu\nu} = 0$), the same equation does not contain velocities. Thus, we again have the situation that there are certain equations that can appear either in the form of a dynamical equation or in the form of a constraint, depending on the gauge one adopts. This is similar to the case of equation (10) or (11). As we have outlined above, such intermediate equations are lost during the reduction process. We should point out, however, that there are certain restrictions concerning the above gauge choices. For instance, it has been argued in [10] that the gauge $\pi = 0$ can be imposed in asymptotically flat spacetimes, but not in finite spaces with non-vanishing curvature. (It is actually quite a general feature of general relativity that the procedure frequently depends right from the start on the solutions one wishes to obtain at the end of the day. We will encounter this feature in more detail in the following sections.)

In summary, there seems to be strong evidence that the constraints (together with the trivial dynamical equations) do not contain the complete physical information and that there is again some kind of interrelation between $N, N_\mu$ (or $g_{0\mu}, g_{00}$) and some (or one) of the gauge variables contained in the non-TT parts of $\pi^{\mu\nu}$ and $g_{\mu\nu}$.

Nevertheless, one should not take the above considerations too seriously. There are fundamental issues that we have not discussed. For instance, the relation to the linear theory
is not really as straightforward as one might think. This is already obvious from the fact that the linearized Hamiltonian (2) can certainly not be obtained by linearization of the full Hamiltonian of general relativity, which is zero, but rather emerges from the second-order terms of the constraint $\mathcal{H}$, taking $N = 1 + h_{00}/2$. Also, there is the matter of the occurrence of a surface term in (16) that we have omitted for simplicity. Another issue concerns the difference of the boundary conditions between conventional gauge theories and general relativity. For instance, one could argue that, in contrast to electrodynamics, the latter admits solutions that are fundamentally non-static and nevertheless are free of radiation (cosmology). Most importantly, however, there is a fundamental difference between the coordinate transformations of general relativity and the corresponding gauge transformations in the linear theory. In that context, there are at least two issues that have to be considered, namely the construction of physical (gauge-invariant) quantities and the special role of the time coordinate. These issues have been intensively studied in the literature on quantum gravity, and it remains for us to see to what extent they affect our specific discussion.

In any case, it turns out that for simple models, like the Robertson–Walker cosmologies we will analyze in the following sections, the situation is the same as in the spin-2 theory, meaning that there is again an equation that is neither part of the dynamical equations nor part of the constraints, and is nevertheless physical in the sense that it is necessary in order to describe the configuration completely.

4. Robertson–Walker cosmologies

We start from the Lagrangian

$$L = -\frac{6R}{N} R^2 + \frac{R^3}{2N} \dot{\phi}^2,$$

which leads to the field equations for a homogeneous, massless scalar field $\varphi = \varphi(t)$ in the spatially flat Friedmann–Robertson–Walker spacetimes

$$ds^2 = N(t)^2 dt^2 - R(t)^2 \delta_{\mu\nu} dx^\mu dx^\nu.$$

For further details, we refer to the study carried out in [11]. For mathematical simplicity, we confine ourselves to flat spaces $k = 0$ and to the massless case $m = 0$, which are explicitly solvable. Obviously, the system of field equations obtained from (17) is underdetermined and has to be supplemented by a gauge choice, e.g., $N = 1$.

The first-order form of the Lagrangian reads

$$L = \pi_R \dot{R} + \pi_\phi \dot{\phi} + N \left( \frac{\pi_R^2}{24R} - \frac{\pi_\phi^2}{2R^3} \right).$$

For the complete analysis of the solutions, we refer to [11]. However, since we will repeatedly have to take square roots of certain variables, it is useful to have in mind the signs of the canonical variables and the velocities. First of all, we can assume $N > 0$ and $R > 0$ (since the original variables, entering the metric, were $N^2$ and $R^2$ anyway). This essentially leaves us with four cases to be considered, which, for our purposes, are conveniently characterized by the signs of $\pi_\phi$ and $\pi_R$.

$$\pi_R > 0, \quad \pi_\phi > 0 : \quad \dot{R} < 0, \quad \dot{\phi} > 0$$

$$\pi_R > 0, \quad \pi_\phi < 0 : \quad \dot{R} < 0, \quad \dot{\phi} < 0$$

$$\pi_R < 0, \quad \pi_\phi > 0 : \quad \dot{R} > 0, \quad \dot{\phi} > 0$$

$$\pi_R < 0, \quad \pi_\phi < 0 : \quad \dot{R} > 0, \quad \dot{\phi} < 0$$
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\[ \pi_R < 0, \quad \pi_\psi < 0 : \quad \dot{R} > 0, \quad \dot{\psi} < 0. \]  

We will mostly deal with case (22), but from a mathematical point of view, the four cases are quite similar.

We note that the action \( S = \int L \, dt \) is invariant under time reparameterizations \( t \rightarrow \tilde{t} \) if \( N \) transforms accordingly, i.e. such that \( N \, dt \) is invariant. What is more interesting for our analysis is the invariance under the gauge transformation induced by the constraint that results from the variation of \( L \) with respect to \( N \), namely

\[ G = \frac{\pi_R^2}{24R} - \frac{\pi_\psi^2}{2R^4} = 0. \]  

Introducing canonical Poisson brackets \( \{\pi_R, R\} = \{\pi_\psi, \phi\} = -1 \), we find that (24) generates the following transformations on the fields and momenta:

\[ \delta R = -\frac{\pi_R}{12R} \varepsilon, \quad \delta \phi = \frac{\pi_\psi}{R^4} \varepsilon, \quad \delta \pi_R = \left( -\frac{\pi_R^2}{24R^2} + \frac{3\pi_\psi^2}{2R^4} \right) \varepsilon, \quad \delta \pi_\psi = 0, \]  

where \( \varepsilon \) is an infinitesimal parameter. Indeed, the Lagrangian (19) is invariant under (25) provided that \( N \) transforms according to \( \delta N = \dot{\varepsilon} \). The above transformation is the remnant of the coordinate transformations \( \delta g_{ik} = g_{ik,m} \xi^m + \xi^m g_{im} + \xi^m g_{mk} \) and \( \delta \phi = \phi,m \xi^m \) of the full theory.

In the following section, we will perform the Hamiltonian reduction of the theory (19) and compare the results, in section 6, with the Wheeler–DeWitt approach as well as with the results obtained from an explicit choice of the time coordinate (section 7) and by a change of variables (section 8).

5. Explicit reduction

Just as in section 2, we will identify the dynamical variables of the theory by the reduction process of Faddeev and Jackiw [3] (which relies on solving the constraint explicitly) and obtain a first-order Lagrangian with a reduced number of variables. In our case, it turns out to be convenient to solve (24) with respect to \( \pi_R \) (although other choices are possible). We find

\[ \pi_R = \pm \frac{\sqrt{12}}{R} |\pi_\psi|, \]  

which again requires the differentiation between the four cases (20)–(23). The Lagrangian is easily put into the form

\[ L = (\phi \pm \sqrt{12} \ln R) \pi_\psi, \]  

where the minus sign (in the following referred to as case 1) holds for cases (21) and (22) and the plus sign (case 2) for cases (20) and (23). (For simplicity, we will not notationally differentiate between the reduced and unreduced Lagrangians in the following sections.)

It is convenient to introduce the variables

\[ X = \phi - \sqrt{12} \ln R, \quad Y = \phi + \sqrt{12} \ln R. \]  

Let us confine ourselves to case 1. Then we have

\[ L = X \pi_\psi, \]  

that is, the dynamical variables are \( X \) and \( \pi_\psi \), and the corresponding Poisson brackets are given by

\[ [\pi_\psi, X] = -1, \quad [X, X] = [\pi_\psi, \pi_\psi] = 0. \]
The Hamiltonian is zero and the classical equations of motion are obviously \( \dot{\pi}_\phi = 0 \) and \( \dot{X} = 0 \). We see that, as has already been stated by Dirac [7], finding the dynamical variables and solving the field equations are essentially one and the same thing in covariant theories.

Since the constraint has been solved for \( \pi_R \), we can now express the transformations (25) in the form

\[
\delta R = \frac{\pi_\psi}{\sqrt{12} R^2} \epsilon, \quad \delta \varphi = \frac{\pi_\psi}{R^3} \epsilon, \quad \delta \pi_\varphi = 0, \tag{31}
\]

and find

\[
\delta X = 0, \quad \delta Y = \frac{\pi_\psi}{R^3} \epsilon, \tag{32}
\]

which confirms that \( X \) and \( \pi_\varphi \) are indeed gauge invariant, as they should, while \( Y \) is a gauge variable. (Note that in case 2, the role of \( X \) and \( Y \) is reversed.)

It is already obvious at this stage that the situation is similar to the spin-2 case. Indeed, from the reduced dynamics that follow from the Lagrangian (29), we can (trivially) determine \( X \) and \( \pi_\varphi \) (just like \( T^{\mu A} \) and \( T^{\pi A} \) in electrodynamics) while the constraint determines \( \pi_R \) (just as it determines the longitudinal part of \( \pi^\mu \) in electrodynamics). Further, the variable \( Y \) is a gauge variable and not of physical interest (just like the longitudinal part of \( A^\mu \) in electrodynamics).

However, from the reduced Lagrangian and from the constraint alone, we cannot determine \( N(t) \). This is again similar to electrodynamics, where \( A_0 \) cannot be determined from the reduced Lagrangian. There is, however, a fundamental difference. In electrodynamics, we do not need \( A_0 \). As we have outlined previously, once we have determined both the longitudinal and the transverse parts of \( \pi^\mu \) (i.e. of the electric field), the first one by the constraint and the second one by the dynamical field equations, and having in addition determined the transverse part of \( A_\mu \) by the dynamical equations, leading to the magnetic field, we have already determined the complete set of gauge-invariant quantities. There is nothing else we need to know. On the other hand, in the present case, even if we fix the variable \( Y \) by choosing a gauge, we still need to know \( N(t) \) in order to determine the spacetime geometry completely. Alternatively, we could fix \( N \) to, say, \( N = 1 \), leaving us with an undetermined \( Y \), and again to an undetermined geometry (since we need both \( X \) and \( Y \) to determine \( R \)).

In other words, there are physically relevant quantities that cannot be determined by the dynamical equation and the constraints alone. It is not hard to show that, for instance, the trace of the Einstein equations, \( G^{\hat{k}}_{\hat{k}} = T_{\hat{k}}^{\hat{\cdot} \hat{\cdot} \hat{k}} \), involves both \( Y \) and \( N \). This equation, which can be derived from (19), but not from the reduced Lagrangian, still remains non-trivial, even if we fix the gauge by fixing \( N \) or \( Y \) (explicitly or implicitly). More explicitly, the equation obtained from the variation of (19) with respect to \( R \), using \( \dot{\pi}_\varphi = 0 \) and the expression for \( \pi_R \) (here for case 1), can be brought into the form

\[
0 = \pi_\psi \sqrt{12} R^2 R - N \pi_\varphi^2, \tag{33}
\]

and is easily shown to be invariant under (31) and \( \delta N = \dot{\epsilon} \). Even if we fix \( N \) to, e.g., \( N = 1 \), the equation still contains both \( X \) and \( Y \), meaning that it is not determined by the dynamical variables \( X \) and \( \pi_\psi \) only. A similar situation holds for the gauge choice, e.g., \( R = t \).

Thus, just as in the linear spin-2 theory, we have a physical (i.e. gauge-invariant) relation between non-dynamical variables, namely between \( N \) and \( Y \). Another line of argumentation is to consider the equation \( \dot{Y} = N \frac{\pi_\varphi}{R} \), which can also be derived from (19). Since \( Y \) is a gauge variable, \( Y \) can be transformed to a constant (or at least to some expression of \( t \) and of the field variables, see section 8). Thus, depending on the gauge one adopts, this equation can occur both in the form of a constraint (i.e. not involving velocities) and in the form of a (seemingly) dynamical equation for \( Y \). As outlined previously, the reduction process, which is based on
solving the (true) constraints and reducing the theory to the truly dynamical (gauge-invariant) variables, has no place for such an intermediate case. Reference to the initial, unreduced Lagrangian therefore cannot be avoided. We will see the consequences of this feature later on.

Let us return to the reduced Lagrangian (29). Having identified the dynamical variables, the transition to the quantum theory is straightforward. We replace the dynamical variables with operators satisfying the commutation relations

\[ i[\pi_\psi, X] = 1, \quad i[X, X] = i[\pi_\psi, \pi_\psi] = 0, \] (33)

which can be explicitly realized with \( X \) a multiplication operator and 

\[ \pi_\psi = -i \frac{\partial}{\partial X}. \] (34)

Since the Hamiltonian is zero, the Schrödinger equation on the state functional (which, in the homogeneous case, is simply a wavefunction), \( H \psi(X, t) = i \frac{\partial}{\partial t} \psi(X, t) \), reduces to \( \frac{\partial}{\partial t} \psi(X, t) = 0 \), i.e. \( \psi \) does not explicitly depend on the time coordinate. In other words, the wavefunction may be any function of \( X = \varphi - \sqrt{\frac{1}{12} \ln R} \),

\[ \psi = \psi(X) = \psi(\varphi - \sqrt{\frac{12}{12}} \ln R), \] (35)

subject to suitable boundary conditions. This is the main result of this section. Obviously, in case 2, where \( \pi_\varphi \) and \( \pi_R \) are both of the same sign, we have a similar result, namely \( \psi = \psi(Y) = \psi(\varphi + \sqrt{\frac{12}{12}} \ln R) \).

Equation (34) is all we get from the canonical procedure. Everything else has to be obtained from purely physical considerations. This concerns in particular the exact definition of the Hilbert space and the boundary conditions, but even if this is done, there remains the fundamental question which \( \psi \) one should actually choose in order to get a reasonable description of the situation. It can hardly be expected that \( \psi \) is completely determined by the boundary conditions alone.

As a final remark, we note that there is only one quantum degree of freedom in the theory. This is of course the result of the very restricted ansatz (18) and \( \varphi = \varphi(t) \). Whether we attribute this degree of freedom to the gravitational field or to the scalar field is a matter of convention (recall that \( X = \varphi - \sqrt{\frac{12}{12}} \ln R \)), although the attribution to the scalar field seems more natural. (One can argue, for instance, that in the absence of the scalar field, no dynamical degree of freedom would remain in the theory.) In the full theory (general relativity with scalar field), we would end up with three pairs of canonically conjugate dynamical variables and attribute two of them to the gravitational field. Convenient examples for studying such systems explicitly are given by the generalized homogeneous cosmologies described, e.g., in [12].

There is one important point we have omitted in our discussion. Solving equation (26), we have assumed that we deal either with one or with the other type of classical solutions. The corresponding quantum theory is described by a wavefunction either in the form \( \psi(X) \) or in the form \( \psi(Y) \). However, there is no need to restrict the quantum theory to specific types of classical solutions (although, of course, a very important restriction has already been made by starting with the specific metric (18)). This means that actually we have to admit both types of solutions. In other words, invoking the superposition principle, we can conclude that the most general wavefunction is of the form \( \psi = \psi_1(X) + \psi_2(Y) \). Therefore, strictly speaking, the reduction procedure is not completely consistent in the way it has been presented above. In particular, if we allow for these mixed types of solutions, we cannot actually identify the physical variables. For instance, the gauge transformations (25) cannot be written in the form (31) (because the solution of the constraint is not unique), and thus the variation of \( X \) and \( Y \)
under gauge transformations will be proportional to the two roots of the constraint equation, meaning that it remains unspecified which of both variables is actually gauge invariant. As a result, one cannot reduce the theory to its two dynamical degrees of freedom \( \pi_\varphi \) and \( X \) and should rather work with four operators instead. In this sense, the Wheeler–DeWitt approach, to which we turn now, is preferable, because it does not require us to determine the classical roots of the constraint equation.

6. Operator ordering in the Wheeler–DeWitt equation

We now compare the results of the previous section with the conventional approach to canonical gravity, where the constraints are not solved, but imposed on the quantum states \([7, 10]\). We thus treat \( R, \pi_R \) and \( \varphi, \pi_\varphi \) as canonical pairs of variables and introduce the corresponding quantum operators, again choosing multiplication operators for \( \varphi \) and \( R \), as well as \( \pi_R = -i \partial_{\pi_R} \) and \( \pi_\varphi = -i \partial_{\pi_\varphi} \). As before, the Hamiltonian (on the constraint surface) is zero, and thus the wavefunction \( \psi(R, \varphi) \) does not explicitly depend on the time coordinate. The dynamics are now described by the so-called Wheeler–DeWitt equation obtained by imposing the constraint (24) on the state

\[
\left( \frac{\pi_R^2}{24R} - \frac{\pi_\varphi^2}{2R^3} \right) \psi(R, \varphi) = 0.
\]  

A major problem concerns the operator ordering in the first term. This issue, in the general framework of canonical gravity, has been addressed many times in the literature, see \([13–18]\), and solutions have been proposed, based on Hermiticity arguments and the requirement that the quantum algebra of the constraints be isomorphic to the classical algebra. To end up with a unique factor ordering, the authors of \([15, 16]\) further require invariance under field redefinitions \( g_{\mu\nu} \to \tilde{g}_{\mu\nu}(g_{\lambda\kappa}) \). A common feature of these argumentations is that the justification of a specific choice of factor ordering is based on the explicit construction of a scalar product in the Hilbert space of the state functionals, since prior to this, any discussion on Hermiticity is meaningless.

However, in our specific case, it turns out that, in view of the results of the previous section, the order of the operators occurring in (36) is already determined uniquely, and no further arguments are required. Indeed, if the Wheeler–DeWitt equation is required to do what it is supposed to do, namely to eliminate the non-physical degrees of freedom from the theory (and not to impose conditions on the physical degrees of freedom), then it should be identically satisfied for the solutions of the state function derived in the previous section, which are physical by construction.

For simplicity, we again restrict ourselves to case 1, where \( X \) is the physical variable and \( Y \) the gauge variable, but the analysis can be straightforwardly generalized to the mixed case. According to the results of the previous section, any function of \( X \) should identically satisfy the Wheeler–DeWitt equation. Expressed in the variables \( R, \varphi \), this means that

\[
\left( \frac{\pi_R^2}{24R} - \frac{\pi_\varphi^2}{2R^3} \right) \psi(\varphi - \sqrt{12 \ln R}) = 0.
\]  

identically, with \( \pi_R = -i \partial_{\pi_R} \). It is not hard to show that, up to equivalent orderings, this requires the Wheeler–DeWitt equation to be written in the form

\[
\left( \frac{1}{24R^3}(R\pi_R \pi_R) - \frac{\pi_\varphi^2}{2R^3} \right) \psi(R, \varphi) = 0.
\]  

(38)
An equivalent ordering is, for instance, \((\frac{2}{M^2} (\pi^2_R - \pi_R \frac{1}{2} \pi_R) - \frac{\pi^2_R}{\pi_R}) \psi(R, \varphi) = 0\). Any other (i.e. inequivalent) ordering would lead to a quantum theory that is inequivalent to the theory obtained from the direct reduction of the Lagrangian to its physical degrees of freedom, as described in section 5. The ordering (38) can indeed be found in the literature, see for instance [19], but on the other hand, it differs, e.g., from the choice adopted in [10], which is \(\sim R^{-1/2} \pi_R R^{-1/2} \pi_R R^{-1/4}\), as well as from the one adopted in [20], which is \(\sim R^{-1/2} \pi_R R^{-1/2} \pi_R\). Not only is (37) not identically fulfilled with such orderings, but in fact it does not admit any solutions of the form \(\psi(\varphi - \sqrt{12} \ln R)\) at all.

Once we have fixed the operator ordering, we can explicitly solve the Wheeler–DeWitt equation, and we find the general solution

\[
\psi(R, \varphi) = \psi_1(R - \sqrt{12} \ln R) + \psi_2(R + \sqrt{12} \ln R),
\]

where \(\psi_1\) and \(\psi_2\) are arbitrary functions of their arguments. In other words, \(\psi = \psi_1(X) + \psi_2(Y)\). As expected, the Wheeler–DeWitt equation does not distinguish between case 1 (where \(X\) is the dynamical variable) and case 2 (with \(Y\) dynamical), which arose upon choosing between the roots (26) of the constraint, since, just as the classical constraint, the Wheeler–DeWitt equation is insensitive to a sign change of \(\pi_R\) or \(\pi_Y\). But, as we have pointed out at the end of the previous section, this is actually a good feature, because the reduction process is not unambiguous and therefore one should allow for both types of solutions \(\psi(X)\) and \(\psi(Y)\), and thus also for superpositions \(\psi = \psi_1(X) + \psi_2(Y)\).

On the other hand, since an initial solution \(\psi(X)\) will remain in this form at all times, we can also consider the restriction of the theory to case 1, as we did in the previous section. Then we know that \(X\) is the physical variable and that the solutions \(\psi(Y)\) have to be excluded. Since this cannot be done by the Wheeler–DeWitt equation, one will have to impose suitable boundary conditions on equation (38) such that only the solutions \(\psi = \psi(X)\) survive.

Another way is to allow for all the solutions, but to take care that the \(\text{unwanted solutions} \quad \psi(Y)\) do not contribute to physical quantities (e.g., expectation values). Indeed, it turns out that, if physical equivalence to the approach of the previous section is to be obtained, the construction of the scalar product in the Wheeler–DeWitt approach is essentially fixed. In the reduced theory described by (29), an obvious choice consists of

\[
\langle \psi_1(X), \psi_2(X) \rangle = \int \psi_1^* \psi_2 \, dX,
\]

where the integration can be taken over the complete set of real numbers (or an appropriate subset, we do not deal with the details here, but confine ourselves to a brief outline of the line of argumentation). Note that if we impose as boundary conditions that the wavefunctions \(\psi\) vanish at the boundary \(X = \pm \infty\) (or any appropriate boundary), then the momentum \(\pi_\varphi = -i \frac{\partial}{\partial \varphi}\) is Hermitian. The scalar product (40) is trivially invariant, since the gauge variables have already been eliminated from the theory.

On the other hand, in the Wheeler–DeWitt approach, one could start with

\[
\langle \psi_1(R, \varphi), \psi_2(R, \varphi) \rangle = \int \psi_1^* (R, \varphi) \psi_2 (R, \varphi) g(R, \varphi) \, dR \, d\varphi,
\]

where the integration is carried out over a suitable set (e.g., positive real numbers for \(R\) and real numbers for \(\varphi\), and \(g(R, \varphi)\) is a weight function that is chosen such that the scalar product is gauge invariant. Performing a change of variables, we can write

\[
\langle \psi_1(X, Y), \psi_2(X, Y) \rangle = \int \psi_1^* (X, Y) \psi_2 (X, Y) \tilde{g}(X, Y) \, dX \, dY.
\]

For the particular functions \(\psi = \psi(X)\), the scalar product (42) reduces to the form (40) if we choose \(\tilde{g} = \tilde{g}(Y)\) satisfying \(\int \tilde{g}(Y) \, dY = 1\).
The major problem with such constructions is the fact that they are only valid for the theory that is confined to the classical solutions of type 1. In case 2, the role of $X$ and $Y$ is to be reversed. However, since there is no need for the physical wave solutions to be in a pure state $\psi(X)$ (or $\psi(Y)$), we have to generalize to the case where both $\psi(X)$ and $\psi(Y)$ can contain physical contributions. In other words, since we actually cannot specify whether the physical variable is $X$ or $Y$, we simply cannot exclude one or the other set of solutions of the wavefunction. A scalar product for mixed functions $\psi(X,Y)$ that reduces to the above in the pure case $\psi = \psi(X)$ or $\psi = \psi(Y)$ can be constructed in the form

$$\langle \psi_1(X,Y), \psi_2(X,Y) \rangle = \int \psi_1^*(X,Y) \psi_2(X,Y) \left[ \delta(X-x_0) + \delta(Y-y_0) \right] \, dX \, dY,$$

where $x_0$ and $y_0$ are suitable constants (or eventually infinite) and from the solutions of the Wheeler–DeWitt equation, we can select the physical parts by imposing suitable boundary conditions (e.g., imposing $\psi(x_0, Y) = 0$ leaves us with $\langle \psi_1, \psi_2 \rangle = \int \psi_1^*(X, y_0) \psi_2(X, y_0) \, dX$, which is of the form (40)).

The relation to the invariant scalar products presented in the literature, see, e.g., [10, 17, 18], is not obvious and remains to be examined. In particular, we should note that it is not at all obvious that one should start with the form (40) in the reduced theory. Other choices are possible and lead to different results in the corresponding Wheeler–DeWitt product, with, e.g., $\rho(R, \phi)$ given in terms of a differential operator instead of a function. The choice of the scalar product is a highly non-trivial matter and we refer to the literature for details, see, e.g., [21]. Our intention is merely to show that one could start the discussion from the explicitly reduced theory, whose structure is much simpler, and then try to derive the corresponding form of the scalar product in the Wheeler–DeWitt approach by requiring consistency with the reduced theory.

Although in the full theory, the complete reduction cannot be performed explicitly, there is an alternative way to reduce the theory to its physical degrees of freedom, which is by fixing the gauge. Again, this is not really a trivial matter and, in general, the allowed gauges can depend on the topological properties of the solutions one wishes to obtain, but at least one does not need the explicit solutions, in contrast to the reduction approach of section 5. Therefore, in the following section, we will illustrate this procedure for our simple model and compare the results with those obtained until now.

7. Time coordinate fixation

There are several natural choices for the time coordinate, all having advantages and limitations. We refer to [11] for a more detailed analysis and confine ourselves to a brief outline of two specific examples. In order to avoid case differentiations, we assume, throughout this section, that the solutions are of type (22), that is, of case 1 with $\dot{R} > 0$.

First, we choose $R = t^{1/3}$. Before we reduce the theory, we have to make sure that this choice of gauge is maintained throughout the evolution of the system, i.e. we must require

$$\frac{d}{dt}(R - t^{1/3}) = \frac{\partial}{\partial t}(R - t^{1/3}) + [R - t^{1/3}, H] = 0,$$

where $H$ is the unreduced Hamiltonian found in (19), i.e. $H = -N\left(\pi_R^2 - \pi_\phi^2 \right)$. This leads to $N = -4t^{-1/3} / \pi_R$. Solving the constraint for $\pi_R$, namely $\pi_R = -\sqrt{12} \pi_\phi / R$, we find $N = \frac{3}{2} \pi_\phi$. Since $\pi_\phi$ is a constant of motion (see below) we find that $N$ is constant, meaning that the specific time coordinate can be identified with what is usually called the cosmological time. This is the reason for our specific gauge choice $R = t^{1/3}$,
which, for the rest, does not fundamentally differ from the choice \( R = t \) that has been used in [11].

We point out once again that the determination of \( N \) is needed in order to determine the complete geometry. Leaving out the above step and directly passing over to the reduced theory would result in a loss of information, since \( N \) cannot be determined either by the constraint or by the dynamical equations. The knowledge of \( N \) is certainly of physical interest. Without \( N \) we cannot, for instance, determine the (four-dimensional) curvature scalar. In electrodynamics, one can proceed similarly, namely, impose, e.g., the Coulomb gauge \( A^{\mu},_{\mu} = 0 \), and then require that the gauge is maintained in time, i.e. \( [H, A^{\mu},_{\mu}] = 0 \). This leads to \( \Delta \lambda_0 = 0 \). In contrast to the present case, however, this step is actually not required, because we do not need to know anything about \( A_0 \). As argued before, both the electric and the magnetic fields are fully determined by the constraints \( \pi^{\mu},_{\mu} = 0 \) and by the dynamical equations for the transverse fields. (The only purpose of the above step is to check for consistency, i.e. to check whether one is actually allowed to impose \( A^{\mu},_{\mu} = 0 \).)

We can now reduce the Lagrangian (19) by inserting \( R = t^{1/3} \) and the solution of the constraint \( \pi_R = -\sqrt{12} \pi_\psi/R \). We find

\[
L = \pi_\psi \dot{\psi} - \frac{2}{\sqrt{3}} \pi_\psi, \tag{45}
\]

or for the Hamiltonian

\[
H = \frac{2}{\sqrt{3}} \pi_\psi. \tag{46}
\]

Up to a factor \( 1/3 \), this is the same Hamiltonian that one obtains in the gauge \( R = t \), see [11]. From (45), we see that the canonical variables are \( \psi \) and \( \pi_\psi \), and consequently we introduce the multiplication operator \( \psi \) together with \( \pi_\psi = -i \frac{\partial}{\partial \psi} \). Note by the way that (45) leads to the classical solution \( \pi_\psi = \text{const} \), and therefore \( N = \text{const} \), as outlined above. On the quantum level, the dynamics are described by the Schrödinger equation

\[
H \psi(\psi, t) = i \frac{\partial}{\partial t} \psi(\psi, t), \tag{47}
\]

There is no factor ordering problem in that equation, and upon introducing a new variable \( \tau = \sqrt{12} \ln t^{1/3} \), one finds \((\partial_\psi + \partial_\tau)\psi = 0\), i.e. \( \psi = \psi(\psi - \tau) \). In other words, the general solution of (47) reads

\[
\psi(\psi, t) = \psi(\psi - \sqrt{12} \ln t^{1/3}), \tag{48}
\]

which, for \( R = t^{1/3} \), is fully consistent with the results (35) obtained from the direct reduction. In this gauge, it is particularly obvious that the dynamical degree of freedom is contained in the scalar field and not in the geometry. Similar to section 5, the reduction to (45) is not unique (there are two roots to the constraint equation), and thus the above solutions have to be completed by adding the contributions of the form \( \psi(\psi, t) = \psi(\psi + \sqrt{12} \ln t^{1/3}) \).

Since (47) is free of ordering problems, we could have equally well used this particular gauge in order to determine the correct ordering that has to be adopted in the Wheeler–DeWitt equation. The fact that in the specific gauge the theory is free of ordering problems turns out to be a coincidence and is not a general feature, as we will see in our next example.

Let us consider the gauge \( \varphi = t \). Again, we have to require that the gauge is maintained throughout the evolution, similar to (44), before we solve the constraint. This is easily done and leads to \( N = R^{3}/\pi_\psi \), which, for classical solutions, leads to an exponential behavior \( N \sim \exp(\sqrt{3} t/2) \). Next, we reduce the Lagrangian, inserting \( \varphi = t \) and solving the constraint (conveniently for \( \pi_\psi \) this time). The result is

\[
L = \pi_R \dot{R} - \frac{1}{\sqrt{12}} R \pi_R, \tag{49}
\]
and thus the Hamiltonian reads
\[ H = \frac{1}{\sqrt{12}} R \pi R, \] (50)
which is time independent this time, but not free of ordering problems. With the multiplication operator \( R \) and \( \pi R = -i\partial_R \), we write the Schrödinger equation in the form
\[ -i \frac{1}{\sqrt{12}} R \frac{\partial}{\partial R} \psi(R, t) = i \frac{\partial}{\partial t} \psi(R, t), \] (51)
which has the general solution \( \psi(R, t) = \psi(t - \sqrt{12} \ln R) \), consistent with (35) and \( t = \varphi \).

Note that this result has been obtained using the particular ordering (50) and not, e.g., the symmetric ordering \((1/2)(R\pi R + \pi RR)\) that is conventionally adopted. Any ordering different from the above would lead to results that are not equivalent to those obtained in the reduced theory or to those obtained in the gauge \( R = t^{1/3} \), which were both free of ordering problems.

One might argue that \( H \) is not Hermitian with the above ordering. This, however, is again related to the question of the construction of the scalar product. Indeed, the above Hamiltonian suggests the use of the form
\[ \langle \psi_1, \psi_2 \rangle = \int \psi_1^* (i\partial_R) \psi_2 \, dR, \] (52)
with suitable integration boundaries, at which the wavefunction is assumed to vanish. This product satisfies the usual properties of a scalar product except that it is not positive definite.

We can now show that \( H \) from (50) satisfies the relation
\[ \langle \psi_1, H \psi_2 \rangle = \langle H \psi_1, \psi_2 \rangle, \] (53)
that is, \( H \) is pseudo-Hermitian. The same holds for \( \pi_R \), but not for \( R \). Nevertheless, \( H \) has complex eigenvalues, as is easily shown by considering an eigenfunction \( \psi_a \) satisfying \( H \psi_a = a \psi_a \) and showing that the state \( R \psi_R \) is again an eigenfunction of \( H \), with the eigenvalue increased by an imaginary amount. This again shows the difficulties in the construction of the scalar product and the interpretation of the wavefunction in general [21].

8. Change of variables

In [16], the question has been raised whether one could eventually circumvent the difficulties with the ordering problems by multiplying the constraint by \( R \) before the transition to the quantum theory. According to the authors, this is not allowed, because the resulting wavefunctions would exhibit radically different behaviors from the original ones. We will demonstrate that in fact, both parts of the statement are not entirely accurate. Namely, we find that multiplication by \( R \) does not resolve the ordering problems, and that the resulting wave equation has exactly the same solutions as in the original formulation, provided a consistent ordering is adopted.

Multiplication of the constraint by \( R \) is essentially the result of a change of variables. Namely, if we introduce a new variable \( \tilde{N} = \frac{N}{R} \), the Lagrangian (19) takes the form
\[ L = \pi R \dot{R} + \pi \psi \dot{\psi} + \tilde{N} \left( \frac{\pi R^2}{24} - \frac{1}{2R^2} \pi \psi^2 \right). \] (54)

This can be explicitly reduced to
\[ L = \pi \psi \dot{X}, \] (55)
with \( X \) as before, where we have solved the constraint assuming again that \( \pi_R \) and \( \pi \psi \) have different signs (case 1). In other words, the dynamical variable is \( X \), and the state function is
a general function \( \psi(X) \). Of course, just as in section 5, the solution of the constraint (and thus the reduction procedure) is not unique, and we have to add contributions of the form \( \psi = \psi(Y) \).

Therefore, if the theory is still consistent, the Wheeler–DeWitt equation

\[
\left( \frac{\pi_R^2}{24} - \frac{1}{2R^2} \pi_Y^2 \right) \psi(R, \varphi) = 0
\]

should be identically satisfied for \( \psi = \psi(\varphi - \sqrt{12} \ln R) \) (and for \( \psi = \psi(\varphi + \sqrt{12} \ln R) \) or a linear combination of both). At first sight, this does not seem possible, and it seems as if (56) is free of ordering ambiguities. However, (56) is indeed identically satisfied for the above solutions if we adopt the ordering \( \pi_Y^2 = \frac{1}{R^2} \pi_R R \pi_Y \). This looks rather unorthodox, but it is actually very similar to the ordering in (38).

We are thus led to the conclusion that \( \pi_Y^2 \) is not an unambiguously defined operator. As a result, we must assume the same for \( \pi_X^2 \), meaning that we actually have not been very careful in section 6, where we have simply assumed that \( \pi_X^2 = \pi_Y \pi_Y \). It is, however, obvious that this is indeed the only possible ordering in the second term of (38) in order for (37) to be identically satisfied.

A more clever choice, rather than just replacing \( N \), is to use the variables \( X, Y \) and \( \tilde{N} = 2R^{-3}N \). The second-order Lagrangian (17) then simplifies to \( L = \frac{1}{\tilde{N}} \dot{X} \dot{Y} \), and the corresponding first-order Lagrangian reads

\[
L = \pi_X \dot{X} + \pi_Y \dot{Y} + \tilde{N} \pi_X \pi_Y.
\]

The analysis is now trivial. We solve the constraint by \( \pi_Y = 0 \) (case 1) or \( \pi_X = 0 \) (case 2), and the Lagrangian reduces to (in case 1) \( L = \pi_X X \), with the dynamical variable \( X \) and wavefunctions \( \psi(X) \). On the other hand, in the Wheeler–DeWitt approach, we have to solve the equation

\[
(\pi_X \pi_Y) \psi(X, Y) = 0,
\]

which is, this time, completely free of ordering problems, and directly leads to the solutions \( \psi = \psi_1(X) + \psi_2(Y) \), just as in section 6.

The above choice of variables is essentially the only one that leads to a Wheeler–DeWitt equation without ordering problems (without explicitly fixing the gauge). It is thus clear that in general, where we do not know the explicit solutions of the field equations, we will not be able to find the corresponding form of the Wheeler–DeWitt equation, meaning that such a change of variables cannot be used as a tool to determine the correct ordering that has to be adopted when the same equation is formulated in terms of other variables. The argument nevertheless demonstrates once more that there is indeed a unique factor ordering in order to get a consistent theory, and that it is not simply a matter of a global shift in the energy level shifts, as has been suggested, e.g., in [11].

On the occasion, we also observe that it is not possible to fix the gauge implicitly by imposing a condition \( f(X, Y, \pi_X, \pi_Y) = 0 \) with a time independent \( f \). Indeed, stabilization of such a gauge choice will always lead to an expression proportional to \( \tilde{N} \), which would mean that either \( \tilde{N} \) has to be zero (which we have to exclude) or that we get yet another condition \( g(X, Y, \pi_X, \pi_Y) = 0 \) on the variables. Together with the original Wheeler–DeWitt constraint, this would make three relations between four variables, which is obviously not allowed, since two variables correspond to propagating fields. Thus, any gauge fixation will necessarily depend explicitly on the time coordinate, \( f(X, Y, \pi_X, \pi_Y, t) = 0 \). Since there is no reason to involve the dynamical fields into such a condition, and since \( \pi_Y \) is already zero on the constraint (in case 1), the most natural choices are of the form \( Y = f(t) \) for some function
f(t). Stabilization leads to $\tilde{N}^{-1} = -\pi_X/f(t)$. Conditions of the form $Y + g(X) = f(t)$ lead to the same expression for $\tilde{N}$, since the Poisson bracket of the second term with the Hamiltonian is proportional to $\pi_Y$, which is zero on the constraint surface. In fact, it is obvious that the dynamical variables commute with the constraint anyway, and there is thus no need to include them into the gauge fixing conditions. Nevertheless, in this way one can formally obtain, e.g., the previously used gauges $\psi = t$ or $R = t^{1/3}$. It should be noted that the above argumentation assumes that the solutions are of type 1. In the case where $Y$ is the dynamical field, we obviously cannot use $Y = f(t)$, but should rather use $X = f(t)$. One might therefore think that a better choice would be of the form, e.g., $X + Y = f(t)$, since it covers both cases. This does not solve all the problems, though, as we will see in the following section.

The fact that the operator ordering can be fixed by performing a change of variables such that the resulting equations take a form free of ordering problems was also the starting point of the investigations carried out in [15, 16]. In particular, the authors managed to generalize their arguments to the complete theory.

The form (58) is also particularly convenient for analyzing the classical limit of the theory. Namely, if we write the wavefunction in the form $\psi = a(X, Y) \exp[iS(X, Y)/\hbar]$, with real functions $a$ and $S$, then the Wheeler–DeWitt equation leads to

$$\frac{\partial S}{\partial X} \frac{\partial S}{\partial Y} = \hbar^2 \frac{\partial^2 a}{\partial X \partial Y}$$

(59)

$$\frac{\partial S}{\partial Y} \frac{\partial a}{\partial X} + \frac{\partial S}{\partial X} \frac{\partial a}{\partial Y} = -a \frac{\partial^2 S}{\partial X \partial Y}.$$  

(60)

The first equation, in the limit $\hbar \to 0$, reduces to the Hamilton–Jacobi equation, while the second equation is commonly interpreted as a conservation equation for the probability density. We see in particular that the pure states of the form $\psi = \psi(X)$ or $\psi = \psi(Y)$ are not only the solutions of (59) and (60), but also the exact solutions of the Hamilton–Jacobi equation $\frac{\partial S}{\partial X} \frac{\partial S}{\partial Y} = 0$. Only for mixed solutions $\psi = \psi(X) + \psi(Y)$ will the quantum corrections in (59) be effective. The same analysis is easily performed in the original variables $R$ and $\phi$, where one can also directly verify that the Hamilton–Jacobi limit does not depend on the operator ordering.

9. Discussion

The analysis of the simple cosmological models allows us to identify a direct consequence of the fact that the theory is not completely determined by the constraints and by the dynamical equations alone. That this is the case, we repeat, can simply be recognized by the fact that we have five variables in the theory, $\phi, \pi_\phi, R, \pi_R, N$, two of which are dynamical, one is eliminated by the constraint and one can be fixed by imposing a gauge. This leaves one undetermined variable. However, once the time coordinate has been chosen, the metric should be determined completely. The missing relation can only be obtained from the unreduced Hamiltonian, for instance by stabilization of the gauge fixing condition. But this turns out to lead to an astonishing feature of the theory.

Indeed, since we concentrated on the dynamical variables, we have glanced over a particularity of the theory. To be explicit, we consider the case where the time coordinate is chosen as $R = t^{1/3}$, but similar arguments apply to any other gauge choice.

We have shown that stabilization of the gauge $R = t^{1/3}$ leads to $N = \frac{2}{\sqrt{3} \pi_X}$, from which we concluded that, since $\pi_\phi = 0$, $N$ has to be a constant. This is true on the classical level,
but it is not entirely accurate in the quantum theory. Indeed, since in the specific gauge, \( \varphi \) and \( \pi_\varphi \) are the dynamical fields of the theory, we have to interpret the above relation as an operator equation. Little attention has been given to this particularity of gravity in the literature, although it has been explicitly mentioned in [10]. Multiplying from the right by \( \pi_\varphi \) and from the left with \( N^{-1} \), we can write

\[
N^{-1} = \frac{\sqrt{3}}{2} \pi_\varphi = -i \frac{\sqrt{3}}{2} \frac{\partial}{\partial \varphi}.
\]

Similarly, in the variables of the previous section, and the gauge \( Y = f(t) \), one obtains the operator \( \tilde{N}^{-1} = i \frac{\dot{f}}{f} \frac{\partial}{\partial x} \). Thus, although, for instance for the above choice, \( \pi_\varphi \) (and thus \( N \)) is constant in the classical theory, and we also have \( i[H, \pi_\varphi] = \pi_\varphi = 0 \) in the Heisenberg representation (with \( H \) from (46)), the statement that \( N \) is constant (cosmological time) does not make sense in the Schrödinger picture.

The fact that there is after all a component of the metric that does not behave classically should not be surprising. Since in the specific gauge, the only dynamical variables are \( \varphi \) and \( \pi_\varphi \), while \( R \) is fixed by the gauge choice, it would be rather strange if the remaining variable contained in the metric (18) was also classical. A back-reaction of spacetime to the presence of the quantum field \( \varphi \) should naturally be expected, and it turns out, in our specific case, that this is achieved not by dynamical (quantum) degrees of freedom of the metric (i.e. by the presence of gravitons), but rather by the quantum nature of the lapse function.

It should be noted that this feature is very unique: we have a quantum operator \( N \) that has to be determined by purely classical means, namely by variation of the Lagrangian (prior to solving the constraint), or equivalently by equation (44) (recall that (44) is a classical equation and \([H, R]\) is the Poisson bracket). For instance, there is no Heisenberg equation \( i[H, N] = N \) prior to the determination of \( N \) in terms of \( \pi_\varphi \). One can argue that the same holds, e.g., for \( \pi_R \), which is also determined classically by solving the constraint, but this is a different situation. \( N \) is neither a constrained variable nor a dynamical one (in a strict sense), and it is nevertheless needed to determine the configuration completely. As for \( \pi_R \), it can either be eliminated prior to quantization or, in the Wheeler–DeWitt approach, it remains in the theory, but its relation to the other variables is not given in terms of an operator equation (i.e. the constraint \( \pi^2_R - \pi^2_\varphi = 0 \) applies only to physical states). On the other hand, equation (61) is a true operator equation (see the remarks in [10] on this point).

This particular situation is obviously a result of the fact that the theory is not described merely by the dynamical variables and the constraints and cannot occur in conventional gauge theories. For instance, in electrodynamics, it is possible that \( A_0 \) turns into a quantum operator, for instance through the stabilization of the gauge fixing \( A_{\mu,\nu} = 0 \), which leads in the presence of charged matter to \( \Delta A_0 = \rho \). Since \( \rho \) is gauge invariant, it has to be constructed from the dynamical variables of the matter field, and thus from operators in the quantum theory, e.g., \( \rho = e\bar{\psi}_\psi \). However, this is not physically relevant, since the knowledge of \( A_0 \) is not needed for the description of the theory (what we need instead is the constraint \( \pi_{\alpha,\mu} - \rho = 0 \), which is, however, not an operator relation and applies only to the physical states) and thus we can simply forget about \( A_0 \).

Note that the operator form of \( N \) can only be determined once a specific gauge has been chosen. Prior to this, there is no expression of \( N \) in terms of the remaining fields that does not involve velocities. (Obviously, since if there were, this would mean that there is an additional constraint in the theory.) What we have (for instance, in case 1), is an equation of the form \( \dot{Y} = \frac{\Delta}{\Delta t} \pi_\varphi \) (on the constraint surface). Only if we fix the gauge variable \( Y \), such that \( \dot{Y} \) becomes an explicit function of the field variables and \( t \), can we derive the explicit form of the operator \( N \).
We should point out that there is actually an additional problem. In fact, since the reduction is not unique, and we cannot actually decide which are the physical variables, we do not really know which are the allowed gauge choices. As pointed out before, the choice $Y = f(t)$ is only possible in case 1. But even if we assume, for instance, that the choice $R = t^{1/3}$ that we used above is allowed in both cases, leading to $\varphi$ and $\pi_\varphi$ as physical variables, then we still cannot determine the operator form of $N$ without an explicit reference to a specific type of solutions. Namely, fixation of the gauge condition leads, as we have seen, to $N = -4t^{-1/3}/\pi_R$, where $\pi_R$ has to be eliminated with the help of the constraint. This cannot be done uniquely and leads to both solutions $N^{-1} = \pm i\sqrt{3}/\pi_R$; compare with (61). In this particular case, we can simply claim that the ambiguity in the sign is not of any relevance, since the original variable in the metric was $N^2$ anyway. But if we consider, for instance, the variables used in the previous section, and fix the gauge by $X + Y = f(t)$ (which is allowed, since it does not constrain the dynamical variable either in case 1 or in case 2), then stabilization leads to $\tilde{N}^{-1} = -(\pi_X + \pi_Y)/\dot{f}$. One of both momenta is to be eliminated by the constraint, but we cannot determine which one, meaning that we do not know the explicit operator form of $\tilde{N}^{-1}$ before we identify either $X$ or $Y$ as a physical variable (i.e. before we confine ourselves to a particular type of classical configurations).

In particular, although the Wheeler–DeWitt approach was previously very elegant, since it allowed us to directly find the general form of the wavefunctionals without solving the constraint classically, and thus without choosing one of both roots, the problem reappears at the level of the determination of the operator form of $N$. As pointed out before, $N$ can only be determined after a gauge has been chosen, since prior to this, there is no equation for $N$ that does not involve time derivatives. But if we fix the gauge, we are left with three variables, and thus we cannot work with two pairs of canonically conjugated variables (as in the Wheeler–DeWitt approach). Rather, we have to eliminate one of the remaining variables with the help of the constraint and reduce the theory to a single pair of canonically conjugated variables.

Alternatively, one could argue that we do not need the operator form of $N$. Since we already know the solutions for the wavefunction, one could claim that anything else should be determined with the help of that wavefunction. Such an argumentation, however, is hard to support, since we already know that, on the classical level, we need to know $N(t)$ (once the gauge is fixed), and therefore if we omit it completely on the quantum level, then we also lose the possibility of recovering the classical limit. In fact, in [22], a theorem has been proven which states that from the Hamilton–Jacobi limit of the Wheeler–DeWitt equation, we can derive the classical Hamiltonian equations for the canonical fields $\pi^{\mu\nu}$ and $g_{\mu\nu}$, and that if these are satisfied, there exist functions (lapse and shift) $N$ and $N_\mu$ such that the metric $g_{\mu\nu}$ (constructed in the usual way from $g_{\mu\nu}$ and $N$, $N_\mu$) satisfies the Einstein field equations. The functions $N$ and $N_\mu$ themselves, however, are not specified by the Hamilton–Jacobi equation. (This means that, even if we fix the coordinate system by imposing conditions on the non-propagating components of $\pi^{\mu\nu}$ and $g_{\mu\nu}$, the metric will not be determined completely.)

Finally, we present a few speculations concerning the reason for these specific features of general relativity. One could think that this feature of gravity is a result of the reparameterization invariance. However, as we have seen, we have a similar situation in the special relativistic spin-2 theory, which is not reparameterization invariant, and on the other hand the special relativistic point-particle Lagrangian, which is reparameterization invariant, does not share the same features, see [1]. In fact, in the latter case, the role of $N$ is played by a Lagrange multiplier $\lambda$, which is introduced by hand and is thus trivially unphysical. Thus, if we choose, e.g., the gauge $\tau = t$ ($\tau$ is the parameter of the theory, $S = \int L \, d\tau$, see [1]), then the stabilization of the constraint merely leads to the determination of $\lambda$, which is
completely uninteresting, while the dynamical variables determine the position $x^\mu$ in terms of $t$.

Since the reason cannot be found either in the general covariance or in the reparameterization invariance nor in the nonlinearity of the theory, where can it be found? The only common feature of the linear spin-2 theory and general relativity we can think of is the fact that they are spin-2 theories. By (massless) spin-2 theory, we mean a theory whose first-order approximation leads to a wave equation for a symmetric, traceless-transverse tensor field, and is, in addition, Lorentz invariant. Note that in the case of general relativity, this requires reference to a fixed background metric. We believe that the reason behind the fact that both general relativity and linear theory are not completely described by the constraints and the dynamical variables (i.e. by the spin-2 field) alone is that they are more than just spin-2 theories, that is, they are not determined by the mere fact that they are spin-2 theories. Otherwise stated, the spin-2 theory is not unique. This is obvious, since we have already mentioned two different theories, but there are actually more. For instance, one could start from a special relativistic theory based on a traceless field $h_{ik}$ (traceless in four dimensions, in order to retain Lorentz invariance). Similarly, a modification of general relativity based on a metric that satisfies $\det g_{ik} = -1$ (the so-called unimodular theory, see [23, 24]) still leads to a spin-2 theory.

The important thing is that these theories are all based on different gauge groups, meaning that the requirement of a theory to describe a spin-2 particle does not uniquely fix the symmetry group. On the other hand, there is only one possible gauge group for the spin-1 theory. Indeed, if we stick to linear theories, then the only possible form of the reduced Hamiltonian is given by (14), and the only Lorentz invariant theory that leads to (14) is the conventional Maxwell theory. (Of course, one could start with a field satisfying the Lorentz gauge $A_i^\prime, i = 0$ from the outset, but that leads to an equivalent theory.) Moreover, it has been shown in [25] that the only nonlinear generalizations of the Maxwell theory necessarily admit the same gauge group as the linear theory. (Only if we admit several spin-1 fields, as is the case in the Yang–Mills theory, will the gauge group be modified by higher order terms.)

In the spin-2 case, the situation is different. Even if we start from the symmetry group of the conventional theory, namely $\delta h_{ik} = \xi_{i, k} + \xi_{k, i}$, the nonlinear generalizations can admit either the same symmetry transformations or alternatively the symmetry transformations of a generally covariant theory, see [25]. Moreover, one can start from a linear theory with a reduced symmetry, like the one mentioned before (where $h_{ik}$ is traceless and $\xi_i$ has to satisfy $\xi_i^\prime, i = 0$) and still end up with a spin-2 theory, which is, however, not equivalent to the original one. Thus, although in the conventional theory, we can always choose a (Lorentz covariant) gauge where $h_i^\prime = 0$, imposing this from the outset does not lead to the same theory, quite in contrast to the above-mentioned gauge $A_i^\prime, i = 0$ in electrodynamics. The nonlinear extension of such a traceless theory leads to theories admitting either the same gauge group or the gauge group of unimodular gravity. Note that in general relativity, the situation is similar to the linear theory, namely we can always choose a coordinate system such that $\det g = -1$, but imposing this from the start (i.e. working with a reduced number of fields) leads to a different, inequivalent theory. (We should note, however, that in the linear case, the theory based on the traceless field, although mathematically different, is physically equivalent to the conventional theory, since the reduced Bianchi identities fix the trace of the field equations to a constant. With the conventional boundary conditions of special relativistic theories, this constant can only be zero anyway. In the nonlinear case, the situation is different and we obtain, in the unimodular case, an unspecified cosmological constant.)

We believe that this non-uniqueness of the spin-2 theory is the reason why the theories are not determined by the constraints and the dynamical equations alone. It is not clear to
us though whether this is due to the fact that already a single linear spin-2 theory admits nonlinear generalizations with two different symmetry groups (which is the non-trivial result of the analysis carried out in [25]), or whether it is due to the much simpler fact that there are already several spin-2 theories at the linear level.

10. Conclusions

We have shown that the special relativistic spin-2 theory is not completely specified by the constraints and the equations for the dynamical fields alone. We argued that the same holds in general relativity, and have shown this for simple cosmological examples for which the Hamiltonian reduction can be performed explicitly. While this fact alone is not surprising and is a general feature of gauge theories respectively, in the above cases, we have the situation that there exist gauge-invariant expressions formed with the help of the unspecified variables that cannot be determined without reference to the initial, unreduced Hamiltonian. Thus, in contrast to, e.g., electrodynamics, where both the electric and the magnetic fields are specified by the constraint and the gauge-invariant (transverse) dynamical fields, in the above theories, there are additional gauge-invariant expressions that are not determined by the constraints and nevertheless contain the non-dynamical variables. This concerns, in the spin-2 theory, the trace of the Lagrangian field equations (expressed in terms of Hamiltonian variables), and in general relativity the four-dimensional curvature scalar $4R$ (expressed in terms of Hamiltonian variables). In other words, the invariant equation $4R = 0$ cannot be expressed in terms of the dynamical fields alone (it contains, e.g., the lapse function $N$), nor is it a constraint (it contains, e.g., the velocity $\dot{\pi}$). It therefore cannot be obtained from the explicitly reduced Lagrangian, as we have shown on the example of Robertson–Walker cosmologies.

The situation is not changed if we fix the coordinate system. That is, if we impose gauge conditions on the non-dynamical components of $g_{\mu\nu}$ and $\pi^{\mu\nu}$, the functions $N_\mu$ and $N$ that appear in the expression for $4R$ still remain undetermined. The only way to determine these functions (and thus to obtain the complete set of field equations) is to refer to the initial, unreduced Hamiltonian. Therefore, the equations that determine these functions have to be derived before we actually identify the physical (propagating) variables of the theory. If we stick to the conventional procedure that only propagating variables have to be quantized, this means that the above functions have to be determined by their classical field equations. Once we have established the form $N$ and $N_\mu$ in terms of the remaining fields, we can proceed with the Hamiltonian reduction, identify the propagating fields and quantize the theory. However, since $N$ and $N_\mu$ are now given as expressions in terms of propagating fields (which we can only interpret as operator equations), we have the strange situation that these components are after all quantum operators. In summary, we have quantum operators whose explicit form can only be determined by solving classical equations of motion. While all the above concerning $N$ and $N_\mu$ holds in exactly the same way for, e.g., $A_0$ in electrodynamics, the important thing is that we cannot simply discard the variables $N$ and $N_\mu$ as unphysical gauge variables (as we can with $A_0$), since they are needed in the classical theory to obtain the complete set of coordinate invariant quantities (e.g., the scalar $4R$). If we require the quantum theory to reduce to the classical one in an appropriate limit, it is clear that we need the operator form of $N$ and $N_\mu$. To be precise, we have only shown that the above arguments hold for $N$. It is possible that the expression for $N_\mu$ is not needed, i.e. that for $N_\mu$ we have a situation similar to conventional gauge theories, meaning that there is no gauge-invariant relation that contains $N_\mu$ other than those that are already determined by the constraints and the propagating equations. (Arguments that confirm this will be presented in a subsequent paper, which deals with the so-called invariant representations. As for electrodynamics, the only invariants are the electric
and the magnetic fields, and these are determined completely by the constraint $\pi^{\mu}_{\mu} = 0$ and the equations for the transverse fields $\pi^\mu_{,\mu}$ and $A^\mu_{,\mu}$. No equation containing $A^0$ is thus needed.)

Furthermore, we have shown for the simple cosmological models considered in our analysis that in order to obtain consistency between the explicitly reduced theory and the Wheeler–DeWitt approach, a very specific operator ordering has to be adopted in the Wheeler–DeWitt equation. In contrast to previous arguments, we obtained our result without reference to Hermiticity properties (and thus to the scalar product) and without reference to the classical limit. Although this line of argumentation cannot directly be generalized to the full theory (since the explicit reduction is not possible), it nevertheless shows that the discussion could eventually be carried out independent of the concrete construction of the scalar product.

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