Gauge invariance of the wave functional in mixed momentum/coordinate representations

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Abstract
Starting from the observation that in Yang-Mills theory the Schroedinger state functional in the momentum representation is not gauge invariant, we investigate the reversed question: Which are the representations for the operators of a gauge theory that lead to an invariant wave functional once the quantum constraints have been imposed upon it? Stated otherwise: Which representation do we have to use if we wish the constraints of the theory to eliminate the non-physical degrees of freedom from the states? We use the framework of geometric quantization to attack this question. In particular, it is found that in the linear spin-two theory as well as in General Relativity, gauge invariance cannot be achieved by a pure coordinate (i.e., field) representation, but that one has to use mixed momentum/coordinate representations instead. Our results are illustrated by the example of the free relativistic point-particle as well as by simple cosmological mini-superspace models in the framework of General Relativity.

1 Introduction

The momentum representation is well known as an alternative, but equivalent representation in classical Schroedinger quantum mechanics. Therefore, at first sight, the results presented in [1] and [2] might appear surprising. It is shown for non-abelian Yang-Mills theory that in the conventional coordinate (i.e., field) representation, the state functional is gauge invariant, while this is not the case in the momentum representation. Such an asymmetry between coordinates and momenta is certainly not in the spirit of the Hamiltonian formulation. One is then led to the question whether this is a general feature of gauge theories, or one might speculate that there is something special about the coordinate representation. This is not the case though, and it turns out that the above asymmetry is actually less deep than it appears. Indeed, as far as the physical, unconstrained variables are concerned, there is a complete symmetry between coordinates and momenta, just as we know it from ordinary quantum mechanics, while an asymmetry occurs only as a result of the constraints and therefore affects only the constrained and the gauge variables, but not the dynamical ones.

While this is not hard to recognize, it does still not answer our question. Is the coordinate wave functional generically gauge invariant? More precisely, what one wishes to do, in a gauge theory, is to use a representation where $X$ acts on the states by multiplication ($X$ represents collectively the fields (or the coordinates) of the theory) and the momenta by differentiation, $\Pi = \frac{1}{i} \frac{\delta}{\delta X}$. Then one applies the constraint operator $\hat{G}(X, \Pi)$ on the states $\psi(X)$. The solutions of the equations $\hat{G}(X, \Pi)\psi(X) = 0$ are then expected to be gauge invariant, i.e., to depend only on the gauge invariant components of $X$. In this way, the constraints remove the unphysical degrees
of freedom from the physical states of the theory, a statement that can be found in almost any textbook on quantum field theory. As we have said before, this is true in the Yang-Mills case (and obviously in electrodynamics). It turns out, however, that it is not always true. Consider, for instance, the fourth constraint in the linear spin-two theory, \( h^{ik}_{\cdot,ik} - \Delta h = 0 \). In the quantum theory, this leads to the condition \( (h^{ik}_{\cdot,ik} - \Delta h) \psi(h_{ik}) = 0 \) on the state functional. But in the coordinate representation where \( h_{ik} \) acts by multiplication, this cannot be seen as condition on \( \psi \) (since else, we have to conclude \( \psi = 0 \)), but rather on \( h_{ik} \), i.e., we have to solve the constraint classically such that \( h^{ik}_{\cdot,ik} - \Delta h = 0 \), and then formulate the quantum theory with the remaining components of \( h_{ik} \). This is what one does during the Hamiltonian reduction of the theory, see [3], but it is not what we have in mind here. Here, we wish the constraint itself, as a quantum operator, to eliminate the non-physical variables from the state functional. This is obviously not the case for the above constraint. It is the case for the remaining three constraints of the spin-two theory, \( \pi^{ik}_{\cdot,i} = 0 \), but summing up, we have to conclude that, in the coordinate representation, the constraints do not remove all the unphysical degrees of freedom from the state functional. It is rather obvious what we have to do: For those components of \( h_{ik} \) that appear in the expression \( h^{ik}_{\cdot,ik} - \Delta h \), we have to use a momentum representation and turn them into differentiation operators. Simultaneously then, some components of the momenta \( \pi^{ik} \) will turn into multiplication operators. It turns out that we are lucky inasmuch those specific components do not appear in the expression \( \pi^{ik}_{\cdot,i} \), such that the remaining three constraints still eliminate three degrees of freedom from \( \psi \). Therefore, in this new, mixed coordinate/momentum representation, the constraints do indeed what they are supposed to do, namely they remove the unphysical degrees of freedom from the theory.

Now we have answered our question, namely the coordinate wave functional is not necessarily gauge invariant, but there might be an invariant functional corresponding to a different, possibly mixed, representation. (By invariant functional, we always understand a functional that becomes invariant upon imposing the quantum constraints). All we need now is a systematic way to identify the corresponding representation(s) for general gauge theories. That is the main subject of the present article. A convenient approach to the problem is provided by the formalism of geometric quantization, the basic features of which we present in the next section. Explicit applications are presented in the remaining sections.

2 Geometric quantization

A clear and concise introduction to the formalism of geometric quantization can be found in [2]. The presentation provided there is completely sufficient for our purposes, and there is also no way to present things in a simpler way. For the mere purpose of self-containment of our paper, we will repeat step by step the presentation of [2]. On the occasion, we will introduce a new index notation that we find convenient for our later applications.

We start from a set of canonical coordinates (or fields) \( q^{A} \) and corresponding momenta \( p_{A} \), where \( A \) can be any kind of index, discrete or continuous. By canonical, we mean that the kinetic term in the first order Lagrangian is (up to a total derivative) of the form \( p_{A} \dot{q}^{A} \), resulting in the standard symplectic two-form (see below). For the specific subject we wish to study, it is important to keep track of the momenta and coordinates. Therefore, instead of labeling the phase-space variables with an index running over twice the range of the index of \( q^{A} \), we use a notation of the form

\[
\xi^{A\alpha} = (p_{A}, q^{A}), \quad \alpha = 1, 2.
\] (1)

The symplectic two-form \( \omega = \frac{1}{2}(\omega_{AB})_{\alpha\beta} d\xi^{A\alpha} d\xi^{B\beta} \) then has the components \( \delta_{AB} \varepsilon_{\alpha\beta} \), with antisymmetric \( \varepsilon_{\alpha\beta} \), and \( \varepsilon_{12} = 1 \). This form is exact, \( \omega = d\vartheta \), and thus, we can write

\[
\omega = d\vartheta = \frac{1}{2}(\omega_{AB})_{\alpha\beta} d\xi^{A\alpha} d\xi^{B\beta}, \quad (\omega_{AB})_{\alpha\beta} = \frac{\partial \vartheta_{B\beta}}{\partial \xi^{A\alpha}} - \frac{\partial \vartheta_{A\alpha}}{\partial \xi^{B\beta}} = \delta_{AB} \varepsilon_{\alpha\beta}.
\] (2)
The physical object is $\omega$, while $\vartheta = \partial_{Aa}d\xi^{Aa}$ is only defined up to an exact form. The conventional choice is $\vartheta_{Aa} = (0, p_{A})$, leading to $\vartheta = p_{A}dq^{A}$. Note also that in the case of field theory, partial derivatives have to be replaced by variational derivatives and $\delta_{AB}$ by a delta-function.

Next, to each phase-space function $G(\xi)$, we introduce a corresponding vector field $v(\xi)$ via

$$v^{A\alpha}(\omega_{AB})_{\alpha\beta} = -\frac{\partial G}{\partial \xi^{B\beta}},$$

or equivalently

$$v^{A\alpha} = -\varepsilon^{\alpha\beta}\frac{\partial G}{\partial \xi^{A\beta}}.$$  \hspace{1cm} (3)

The function $G(\xi)$ is also called the generator of the vector field $v(\xi)$, but we will not make use of this vocabulary in order to avoid confusion with the generators of symmetry transformations. Further, for the same quantity $G(\xi)$, we introduce an operator $\hat{G}$ defined as

$$\hat{G} = \frac{1}{i}v^{A\alpha}D_{A\alpha} + G, \quad \text{with} \quad D_{A\alpha} = \frac{\partial}{\partial \xi^{A\alpha}} - i\vartheta_{A\alpha}.$$  \hspace{1cm} (4)

Those operators, referred to as pre-quantized operators, act on the so-called pre-quantized wave functions (or functionals) $f(\xi)$ that vary over the entire phase space, depending thus on both $q^{A}$ and $p_{A}$.

In particular, for the coordinates $q^{A} = \xi^{A1}$, we find from (3) the vector $v^{AB\alpha} = (-\delta^{AB}, 0)$ (there is an additional index on $v$ here, because $G = q^{A}$ already carries an index), and from (4) the operator

$$\hat{q}^{A} = \frac{1}{i} \left[ -\frac{\partial}{\partial p_{A}} + i\vartheta_{A1} \right] + q^{A}.$$  \hspace{1cm} (5)

Similarly, for $p_{A} = \xi^{A1}$, we have $v^{AB\alpha} = (0, \delta^{AB})$ and

$$\hat{p}_{A} = \frac{1}{i} \left[ \frac{\partial}{\partial q^{A}} - i\vartheta_{A2} \right] + p_{A}.$$  \hspace{1cm} (6)

The explicit form depends on the choice of $\vartheta$.

The final step towards the quantum theory is the choice of a so-called polarization. This consists in choosing vector fields $\pi$ which span half the phase-space and imposing the following conditions on the pre-quantized wave functions $f(\xi)$

$$\pi^{BA\alpha}D_{A\alpha}f(\xi) = 0.$$  \hspace{1cm} (7)

For instance, choosing for $\pi^{AB\alpha}$ the vector generated by the coordinates $q^{A} = \xi^{A1}$, i.e., $\pi^{AB\alpha} = (-\delta^{AB}, 0)$, the above condition takes the form

$$D_{A1}f = (\frac{\partial f}{\partial \xi^{A1}} - i\vartheta_{A1})f = 0,$$  \hspace{1cm} (8)

which leads, with the conventional choice $\vartheta_{Aa} = (0, p_{A})$ to $\frac{\partial f}{\partial p_{A}} = 0$, meaning that the function $f(\xi)$ depends merely on the coordinates and not on the momenta, i.e., $f = \psi(q^{A})$. (In addition, $f$ may also depend on time, but we suppress this in our notation.) This corresponds to the coordinate representation. Indeed, it is straightforward to verify that (5) and (6) now reduce to the conventional representations $\hat{q}^{A} = q^{A}$ and $\hat{p}_{A} = \frac{1}{i}\frac{\partial}{\partial q^{A}}$. In the same way, the momentum representation is obtained by choosing for $\pi^{AB\alpha}$ the vector generated by the momenta $p_{A}$, see [2]. We will illustrate this for the example of non-abelian Yang-Mills theory at the end of this section.

Finally, we turn to the study of symmetry generators. Classically, such a generator $G$ induces a change in the phase-space variables $\xi$ via

$$[G, \xi^{A\alpha}] = \frac{\partial G}{\partial \xi^{B\beta}} [\xi^{B\beta}, \xi^{A\alpha}] = \frac{\partial G}{\partial \xi^{B\beta}} (\omega^{BA})^{\beta\alpha} \equiv -\delta_{A\alpha}.$$  \hspace{1cm} (9)
where [,] is the canonical Poisson bracket and \((\omega^{AB})_{\alpha\beta} = -\delta^{AB}\epsilon^{\alpha\beta}\) is the inverse of \((\omega_{AB})_{\alpha\beta}\). In components, we find
\[
\delta q^A = \frac{\delta G}{\delta p_A}, \quad \delta p_A = -\frac{\partial G}{\partial q^A},
\]
which leads, via (3) to the vector field \(v^{A\alpha} = (\delta p_A, \delta q^A) = \delta \xi^{A\alpha} \). (This explains the earlier mentioned vocabulary, namely to call \(G\) the generator of the corresponding vector field \(v\). Here, however, we are interested in those specific \(G\)'s for which \(\delta \xi\) is indeed a symmetry of the theory.) With \(v\) determined, we can construct the pre-quantized operator corresponding to \(G\) and we find
\[
\hat{G} = \frac{1}{i} \left[ \delta p_A \frac{\partial}{\partial p_A} + \delta q^A \frac{\partial}{\partial q^A} \right] - [\delta p_A \vartheta^A_1 + \delta q^A \vartheta_{A2} - G].
\]
(10)

Acting on the pre-quantized function \(f(q^A, p_A)\), we get
\[
\hat{G}f = \frac{1}{i} \delta f - [\delta p_A \vartheta^A_1 + \delta q^A \vartheta_{A2} - G] f = \frac{1}{i} \delta f - [\delta \xi^{A\alpha} \vartheta_{A\alpha} - G] f,
\]
(12)

with \(\delta f = \frac{\partial f}{\partial q^A} \delta q^A + \frac{\partial f}{\partial p_A} \delta p_A\). This is the relation that will be used in all of the following, because it states that, if \(\hat{G}\) is a symmetry operator, then the constraint \(\hat{G}f = 0\) on the wave function leads to \(\delta f = 0\) (i.e., \(f\) gauge invariant) only if \(\delta \xi^{A\alpha} \vartheta_{A\alpha} - G = 0\). Thus, if this is the case, and if we in addition, we use the corresponding representation for which the wave function \(\psi\) of the quantum theory is equal to the pre-quantized wave function after the choice of the polarization (as was the case for the previously presented coordinate representation, \(f = \psi(q^A)\)), then we can conclude that the action of \(\hat{G}\) on \(\psi\) is equivalent to a gauge transformation, and consequently, imposing the constraint \(\hat{G}\psi = 0\) eliminates the unphysical (gauge) degrees of freedom from the theory.

Since there was a double \(i\) in the above argumentation, one might ask whether it is possible for both \(i\)'s to be violated, and the conclusion to be nevertheless true. In other words, can it happen that \(\hat{G}\) is not gauge invariant, and that \(f\) is not equal to the quantum wave function \(\psi\), and that \(\psi\) is nevertheless gauge invariant? This is indeed possible, and is related to the fact that the one-form \(\vartheta\), that appears explicitly in (12), is not uniquely determined, since only the two-form \(\omega = d\vartheta\) is invariant under canonical transformations and thus physically relevant. Therefore, the question whether \(\hat{G}f = 0\) leads to \(\delta f = 0\) or not cannot be of direct physical relevance, since the answer depends on \(\vartheta\). It turns out, however, that a change of \(\vartheta\) by an exact form leads, in the quantum theory, to a shift in the phase of the wave function, and to a corresponding change in the operator representations defined by (5) and (9), such that ultimately, the phase can be discarded and the resulting quantum theory is equivalent to the initial one. Instead of a general proof, we briefly sketch the corresponding issue on the example of non-abelian Yang-Mills theory.

Using the notations of (2), we have the momenta \(p_A = E^i_a\) and the fields \(q^A = A^a_i\). The symmetry generator is given by \((\epsilon^a\) is an arbitrary parameter)
\[
G = \int d^3x \epsilon^a (\partial_i E^i_a + f_{ab}^c A^b_c E^i_c).
\]
(13)

We thus have \(\frac{\delta G}{\delta A^a_i} = f_{ab}^c E^c_i \epsilon^a \equiv -\delta E^i_b\) and \(\frac{\partial G}{\partial E^i_c} = -\epsilon^{ci} + f_{cb}^a A^b_c \epsilon^c \equiv \delta A^i_a\). (The fact that we use the same symbol \(\delta\) both for the change induced by the symmetry generator, e.g., \(\delta A^a_i, \delta f\), etc., as well as for the functional derivatives should not lead to confusion.)

A crucial observation is to recognize that we can write \(G = -\int \delta A^a_i E^i_a d^3x\), and therefore, from (12), we find
\[
\hat{G}f(A, E) = \frac{1}{i} \delta f(A, E) - \int d^3x \left[ \delta E^i_a \vartheta^{a1}_i + \delta A^a_i \vartheta^{a2}_i - \delta A^a_i E^i_a \right] f(A, E).
\]
(14)
First, we make the conventional choice that has also been used in [1], namely $\vartheta^a_1 = 0$ and $\vartheta^a_2 = E^i_a$. We then find immediately $Gf = \frac{i}{2} \delta f$, meaning that once the constraint $Gf$ is imposed, $f$ will be gauge invariant. In the coordinate representation, we have the polarization $D^a_{11} f = 0$, i.e., $\frac{\delta f}{\delta E^a_1} = 0$. Thus, the quantum functional can be chosen to be equal to $f$, and does not depend on $E^i_a$, $f = \psi(A^i_a)$. In particular, $\psi(A^i_a)$ is thus gauge invariant (after imposing the constraint). We can easily check that the operators are in the usual representation, i.e., $\hat{A}^a_1 = A^a_1$ and $E^a_1 = \frac{i}{\sqrt{2}} \frac{\partial}{\partial \vartheta^a_1}$.

On the other hand, the momentum representation is obtained from the polarization $D^a_{12} f = 0$, which leads to $\frac{\delta f}{\delta A^a_1} - i E^a_2 f = 0$, with solution $f = \exp(i \int E^a_2 A^a_1 d^3 x) \varphi(E)$. Hence, we cannot directly use $f(A,E)$ as momentum representation wave functional, but rather, we have to use $\varphi(E)$, which depends only on half of the phase-space variables. Since $f$ was gauge invariant, $\varphi(E)$ is obviously not. This is the result obtained in [1] and [2]. From [6] and [9], we now find the operators $\hat{A}^a_2 = - \frac{1}{2} \frac{\partial}{\partial E^a_2} + A^a_2$ and $\hat{E}^a_2 = E^a_2$. Applied to the above $f$, we see that we can eliminate the phase factor $\exp(i \int E^a_2 A^a_1 d^3 x)$, i.e., we have $\hat{A}^a_2 \varphi(E) = - \frac{i}{2} \frac{\delta}{\delta E^a_2} \varphi(E)$ and $\hat{E}^a_2 \varphi(E) = E^i_a \varphi(E)$ which corresponds indeed to the conventional momentum representation.

It is not unnatural to suspect that the asymmetry between momentum and coordinate representations was brought in by hand, namely when we made the choice $\vartheta^a_1 = 0$ and $\vartheta^a_2 = E^i_a$. In order to show that this is not the case, and that $\vartheta$ can be chosen arbitrarily (provided only that $d\vartheta = \omega$), we now repeat the above analysis with the symmetric choice $\vartheta^a_1 = - \frac{1}{2} A^a_1$ and $\vartheta^a_2 = \frac{1}{2} E^a_2$. This differs from the previous once by a total differential and thus leads to the same symplectic two-form $d\vartheta$. From [14], we now find $\hat{G} f(A,E) = \frac{i}{2} \delta f(A,E) + \int \frac{1}{2} \delta(A^a_1 E^a_2) d^3 x f(A,E)$. We see that now, $f$ is not gauge invariant. Applying again the coordinate polarization $D^a_{13} f = 0$ leads to $\frac{\delta f}{\delta E^a_1} + \frac{i}{2} A^a_1 f = 0$, with solutions $f = \exp(- \frac{i}{2} \int E^a_2 A^a_1 d^3 x) \varphi(A)$. Thus, in the quantum theory, we cannot use $f(A,E)$, but have to use $\varphi(A)$. Also, the operators $\hat{A}^a_2$ and $\hat{E}^a_2$ acting on $f(A,E)$ are modified, but on $\varphi(A)$, they act again as multiplication and differentiating operators, respectively, just as they did in the original coordinate representation on $f(A)$. And finally, we also find $\hat{G} f = \exp(- \frac{i}{2} \int E^a_2 A^a_1 d^3 x) \delta \varphi(A)$, meaning that upon imposing the constraint $\hat{G} f = 0$, we find $\delta \varphi = 0$ and thus $\varphi(A)$ is again gauge invariant. Summarizing, the change of $\vartheta$ by an exact form results in an unphysical phase shift, which can be removed since the operators are modified accordingly, and the resulting wave functional is again gauge invariant. In the same fashion, one shows that for the above $\vartheta$, the wave functional in the momentum representation is again not gauge invariant. The asymmetry between momentum and coordinates is thus not introduced by a specific choice of $\vartheta$ (which is physically irrelevant), but it is a fundamental property of the theory itself. Namely, it enters the theory via the constraint.

Although the choice of $\vartheta$ is physically irrelevant, one would consider the above choice as unwise, in the sense that it only complicates the analysis. If we assume that for a given gauge theory, there exists always a representation for which the wave functional is gauge invariant (after imposing the constraint), then it is obviously preferable to choose $\vartheta$ directly in a way that the pre-quantized functional $f(\xi)$ is already gauge invariant and then look for the representation for which the quantum functional $\psi$ is directly given by the pre-quantized functional after polarization, i.e., $f = \psi$. If instead we start from a pre-quantized functional that is not gauge invariant, it will be hard to find the representation that leads to an invariant functional in the quantum theory.

It is useful to observe that from [6] and [9], one can read off the following correspondence

$$
\begin{align*}
\vartheta^A_1 &= -q^A, \quad \vartheta^a_2 = 0 \quad \text{implies} \quad f = \psi(p_A) \quad \text{in the momentum polarization} \quad D^a_{12} f = 0, \quad (15) \\
\vartheta^A_1 &= 0, \quad \vartheta^a_2 = p_A \quad \text{implies} \quad f = \psi(q^A) \quad \text{in the coordinate polarization} \quad D^a_{11} f = 0.
\end{align*}
$$

Thus, e.g., for the previously adopted choice $\vartheta^A_1 = -\frac{i}{2} q^A$ and $\vartheta^a_2 = \frac{1}{2} p_A$, the quantum functional $\psi$ does not
directly correspond to the pre-quantized functional $f$ in neither the coordinate nor the momentum representation.

This ends our introduction to geometric quantization and we will now consider concrete examples.

## 3 Linear spin-two theory

The first order Lagrangian for the spin-two theory reads

$$L = \int \left[ \pi^{ik} h_{ik} - H(\pi_{ik}, h_{ik}) + h_{0i}(2\pi^{ik} + \frac{1}{2} h_{ik,i,k} + \frac{1}{2} \Delta h) \right] d^3x,$$

where our signature convention is $\eta_{ik} = -\delta_{ik}$ $(i,k = 1,2,3)$, $h = h_i^i$, and $\Delta h = h_{i,k}^i$. The Hamiltonian has the form

$$H = \int \left[ \pi^{ik} \pi_{ik} - \frac{1}{2} \pi^2 + \frac{1}{4} h_{jk,i} h^{ik} - \frac{1}{4} h_{ijk}^m h_{im} h_{jk}^{im} + \frac{1}{2} h_{ik,m} h_{ik}^{m} - \frac{1}{2} h_{ik}^i h_{ik}^k \right] d^3x.$$

The Lagrangian is invariant under the transformations

$$\delta h_{ik} = \xi_{i,k} + \xi_{k,i}, \quad \delta \pi_{ik} = -\varepsilon_{i,k} + \eta_{ik} \Delta \varepsilon, \quad \delta h_{0i} = \dot{\xi}_i + \varepsilon_{i,i}, \quad \delta h_{00} = 2\dot{\varepsilon}.$$

The transformations of $\pi^{ik}$ and $h_{ik}$ are generated by

$$G_\xi = -\int \xi_i 2\pi^{ik} d^3x, \quad G_\varepsilon = -\int \varepsilon [-h_{ik,i,k} + \Delta h] d^3x,$$

corresponding to the constraint equations $\pi^{ik}_{,k} = 0$ and $-h_{ik,i,k} + \Delta h = 0$.

It is convenient to write the canonical fields $h_{ik}$ and $\pi^{ik}$ in the form

$$h_{ik} = \tau h_{ik} + (\eta_{ik} - \frac{\partial_i \partial_k}{\Delta})^\tau h + h_{i,k} + h_{k,i} = \tau h_{ik} + \bar{\tau} h_{ik} + \gamma_{ik}$$

$$\pi^{ik} = \tau \pi^{ik} + (\eta^{ik} - \frac{\partial^i \partial^k}{\Delta})^\tau \pi + \pi^{ik} + \pi^{k,i} = \tau \pi^{ik} + \bar{\tau} \pi^{ik} + \gamma^{ik},$$

where $\gamma_{ik}$ and $\gamma^{ik}$ are transverse and $\tau h_{ik}$ and $\tau \pi^{ik}$ traceless transverse, see [4] for details. The $TT$, $T$ and $V$ components are easily shown to be orthogonal under integration. Note that we now have

$$\delta_\xi h_{ik} = \delta_\xi \gamma_{ik} = \xi_{i,k} + \xi_{k,i}, \quad \delta_\xi \gamma^i = \xi^i$$

$$\delta_\varepsilon \pi^{ik} = \delta_\varepsilon \gamma^{ik} = \Delta \varepsilon h_{ik} - \varepsilon_{i,k}, \quad \delta_\varepsilon \gamma_i = \Delta \varepsilon,$$

where from now on, we denote by $\delta_\varepsilon$ ($\delta_\xi$) the transformations induced by $G_\varepsilon$ ($G_\xi$). The remaining variations are zero, i.e., $\delta_\varepsilon \tau \pi^{ik} = \delta_\varepsilon \pi^{i,k} = \delta_\varepsilon h_{ik} = 0$ and $\delta_\varepsilon \tau \gamma_{ik} = \delta_\varepsilon \gamma_h = \delta_\varepsilon \pi_{ik} = 0$. The Lagrangian can now be written in the form

$$L = \int \left[ \tau \pi^{ik} \tau h_{ik} + 2\tau \pi \gamma_{h} + 2(\pi^{i,k} + \pi^{k,i}) \dot{h}_{i,k} - H + h_{0i}(2\Delta \pi^k + 2\pi^{i,k} + \bar{\tau} \pi^{ik} + \gamma^{ik}) \right] d^3x,$$

with $H = \int \left[ \tau \pi^{ik} \tau \pi^{ik} + 2\tau \pi_{i,k} \pi^{i,k} - 4\tau \pi^{i,k} - \frac{1}{4} \tau \gamma_{h,i} \gamma^{ik} \right] d^3x$. If we wish to reduce the theory by solving the constraints, we find $\gamma_h = \pi_i = 0$, and the theory reduces to its dynamical variables $\tau \pi^{ik}$ and $\tau h_{ik}$ and
can be trivially quantized, see [4, 5, 6]. Here, instead, we wish to follow the conventional Dirac method, which consists in imposing the constraint on the quantum states of the theory, \( \hat{G}_\xi \psi = \hat{G}_\varepsilon \psi = 0 \). This procedure, in electrodynamics and in Yang-Mills theory, has the effect of eliminating the unphysical (gauge) degrees of freedom from the states in the coordinate representation, \( \psi = \psi(A) \) (suppressing again the explicit time dependence in our notation). Here, however, as we have already mentioned in the introduction, this is not the case. Imposing \( \hat{G}_\xi \psi(h_{ik}) = 0 \) leads to \( \psi = \psi(\hat{\tau}h_{ik}, \hat{\pi}) \), while the fourth constraint \( \hat{G}_\varepsilon \psi(h_{ik}) \) acts simply by multiplication. In other words, if we insist on using the coordinate representation, then we have to solve the constraint \( -\hat{\pi}^{i,k} \hbar + \Delta h = 2\Delta h \) classically, eliminating thereby \( \hbar \) before we perform the transition to the quantum theory. This, however, is a reduction in the sense of [3], as we have performed it in [4], but it is not the Dirac procedure.

If we wish to stick faithfully to the Dirac procedure, it is obvious what we have to do: The field \( \hbar \) occurring in the fourth constraint has to be taken in the momentum representation. More systematically, using the formalism of the previous section, we are looking for a pre-quantized functional that is gauge invariant under both \( \hat{G}_\xi \) and \( \hat{G}_\varepsilon \). According to (12), we have

\[
\hat{G}_\xi f = \frac{1}{i} \delta_\xi f - \left( \int [\delta_\xi \pi^{i,k} \theta_{ik1} + \delta_\xi h_{ik} \varphi^{i,k}] \, d^3x - G_\xi \right) f = \frac{1}{i} \delta_\xi f - \left( \int [\delta_\xi h_{ik} \varphi^{i,k}] \, d^3x - G_\xi \right) f \quad (26)
\]

\[
\hat{G}_\varepsilon f = \frac{1}{i} \delta_\varepsilon f - \left( \int [\delta_\varepsilon \pi^{i,k} \theta_{ik1} + \delta_\varepsilon h_{ik} \varphi^{i,k}] \, d^3x - G_\varepsilon \right) f = \frac{1}{i} \delta_\varepsilon f - \left( \int [\delta_\varepsilon \pi^{i,k} \theta_{ik1}] \, d^3x - G_\varepsilon \right) f. \quad (27)
\]

We also note that \( G_\xi \) is linear in \( \pi^{i,k} \), while \( G_\varepsilon \) is linear in \( h_{ik} \), and therefore, we find \( G_\xi = \int (\delta_\xi h_{ik}) \pi^{i,k} \, d^3x \) and \( G_\varepsilon = -\int (\delta_\varepsilon \pi^{i,k}) h_{ik} \, d^3x \). Therefore, it is straightforward to recognize that with the conventional choice \( \vartheta_{ik1} = 0 \) and \( \varphi^{i,k} = \pi^{i,k} \) (that leads to \( f = \psi(h_{ik}) \) in the coordinate polarization), we find that \( f \) (and thus \( \psi \)) is invariant under \( \hat{G}_\xi \), but not under \( \hat{G}_\varepsilon \), in accordance with our earlier observations. An obvious choice that makes \( f \) invariant under both \( \hat{G}_\xi \) and \( \hat{G}_\varepsilon \) is given by \( \vartheta_{ik1} = -h_{ik} \) and \( \varphi^{i,k} = \pi^{i,k} \). But this is not allowed, since it leads to the double value of the symplectic two-form, \( d\theta = 2\omega \). The crucial point is to recognize that not all components, e.g., \( \vartheta_{ik1} \) occur in \( \int \delta_\varepsilon \pi^{i,k} \theta_{ik1} \, d^3x \), since \( \delta_\varepsilon \pi^{i,k} \) contains only transverse parts, and similar for the remaining terms in (20) and (27). Indeed, if we choose

\[
\vartheta_{ik1} = -\left( \eta_{ik} - \frac{\partial \eta_{ik}}{\Delta} \right) \hat{\tau}h = -\tau h_{ik}, \quad \varphi^{i,k} = \tau \pi^{i,k} + \pi^{i,k} + \pi^{k,i} = \tau \pi^{i,k} + \psi^{i,k} - \tau \pi^{i,k}, \quad (28)
\]

then, in view of the orthogonality of the different tensor parts, we find that \( \hat{G}_\xi f = \frac{1}{i} \delta_\xi f \) and \( \hat{G}_\varepsilon f = \frac{1}{i} \delta_\varepsilon f \), and it is also obvious that \( d\theta \) leads to the canonical form \( \omega \). For the existence of the above choice of \( \vartheta \), it is crucial that the constraints are first class. This ensures that, if for instance \( \tau \pi^{i,k} \) occurs in one constraint, then \( \hat{\tau}h_{ik} \) does not occur in the other, and as a result, we have exactly the correct number of independent, orthogonal variables occurring in the generators to make \( f \) invariant under all of the generators and to still guarantee that \( d\theta = \omega \). It is also clear that for the dynamical variables, \( \tau \pi^{i,k} \) and \( \tau h_{ik} \), which do not appear in the constraints, we have the choice to put them into either component of \( \vartheta_{\alpha} \), e.g., as \( \tau \pi^{i,k} \) in \( \varphi^{i,k} \) as above or as \( -\tau h_{ik} \) into \( \vartheta_{ik1} \) (which would lead to a momentum representation). Mixed representations are also allowed for those variables. This reflects again the fact that for the dynamical variables, there is no asymmetry whatsoever between momenta and fields. The asymmetry enters the theory only via the constraints and therefore affects only the constrained variables (\( \hat{\tau}h, \pi^i \)) and the corresponding gauge variables (\( \tau, h_i \)). This is true for any gauge theory. Thus, for instance, if we wish to use a momentum representation in electrodynamics and still have a gauge invariant wave functional, then the obvious thing to do is to put the transverse fields (\( \tau \pi^i, A_i \)) into the momentum representation, and leave the longitudinal fields in the coordinate representation. In the non-abelian case, the situation is more involved, since the physical components of \( A_i^a \) are not so easily identified, see, e.g., [1].
For the transition to the quantum theory, we need to choose a polarization. What we are looking for is of course the polarization that leads to an identification between the pre-quantized functional \( f \) and the corresponding quantum functional \( \psi \). In fact, the polarization, and thus the variables on which \( \psi \) depends, can directly be read off from (28): The momenta are those fields that occur in \( \partial_1 \psi \) and \( \partial_2 \psi \) (i.e., those fields should be represented with differentiation operators), while the coordinates are the conjugate fields. From (28), we then find that \( \psi = \psi(^T \eta h, \eta, ^r \pi) \). In other words, \( \psi \) depends on the gauge variables, and not on the constrained ones. This is obviously the only way in order for the constraints to be able to remove the unphysical variables.

Somewhat more systematically, the above is achieved with the polarization vector

\[
\pi_{lm}^{ik} = \frac{1}{2} \left[ \delta_i \delta_m \delta_k - \eta \frac{\partial \eta}{\Delta} (\eta^{ik} - \frac{\partial \eta^k}{\Delta}) \right], \quad \pi_{lm}^{ik2} = \frac{1}{2} (\eta^{lm} - \frac{\partial \eta^m}{\Delta}) (\eta^{ik} - \frac{\partial \eta^k}{\Delta}).
\]

(29)

Imposing, according to (7), the polarization on the pre-quantized functional, \( [\pi_{lm}^{ik1}D^{ik1} + \pi_{lm}^{ik2}D^{ik2}]f = 0 \), then leads to (the meaning of the symbolic notation is obvious) \( [\gamma(D_{lm1}) + \gamma(D_{lm2}) + \gamma(D_{lm3})]f = 0 \). Since the three operators are orthogonal, each term has to vanish by itself. Explicitly, with \( \partial \) from (28), we find

\[
D_{lm1} = \frac{\delta}{\delta \pi^{lm}} + i \pi_{lm} \quad \text{and} \quad D_{lm2} = \frac{\delta}{\delta \pi^{lm}} - i \pi_{lm},
\]

leading to the ten constraints

\[
\frac{\delta}{\delta \pi^{lm}} f = \frac{\delta}{\delta \pi^{lm}} f = \frac{\delta}{\delta \pi^{lm}} f = 0,
\]

(30)

with solution \( f = \psi(^T \eta h, \eta, ^r \pi) \), or equivalently, \( \psi(^T \eta h, \eta, ^r \pi) \). Finally, we construct the operators

\[
\hat{h}_{ik} = \frac{1}{i} D^{ik1} + h_{ik}, \quad \hat{\pi}^{ik} = \frac{1}{i} D^{ik2} + \pi^{ik}.
\]

Decomposing into orthogonal components, we find

\[
^T \eta h_{ik} = ^T \eta h_{ik}, \quad \hat{h}_{ik} = \gamma h_{ik}, \quad \hat{\pi}^{ik} = -\frac{1}{i} \frac{\delta}{\delta \pi^{ik} h_{ik}},
\]

(31)

\[
^T \pi^{ik} = -\frac{1}{i} \frac{\delta}{\delta \pi^{ik}}, \quad \hat{\pi}^{ik} = \tilde{\pi}^{ik}.
\]

(32)

Imposing the constraints \( \hat{G} \bar{\psi} = \hat{G} \bar{\psi} = 0 \) on \( \psi(^T \eta h, \eta, ^r \pi) \) now leads to \( \frac{\delta \psi}{\delta \pi^{ik} h_{ik}} = \frac{\delta \psi}{\delta \pi^{ik} \tilde{h}_{ik}} = 0 \) and thus to \( \psi = \psi(^T \eta h) \). This is of course identical to the result one obtains from the reduced theory, i.e., if one starts by solving the constraints classically before the transition to the quantum theory, but it has been obtained here following strictly the Dirac method, albeit in a different representation.

Finally, we note that the classical equations of motion obtained from (25) by variation with respect to \( \pi^{ik} \) and \( \eta h \) have the form (on the constraint surface \( \eta h = \pi^{ik} = 0 \))

\[
\Delta h_{0k} + h_{0i,k} - 2 \tilde{\pi}_{ik} - \hat{h}_{i,k} - \Delta h_{ik} = 0 \quad \text{and} \quad \Delta h_{00} - 2 \tilde{\pi} = 0.
\]

(33)

(34)

Those equations are gauge invariant under (19) and determine the multipliers \( h_{00} \) and \( h_{0k} \). What we wish to point out here is the fact that, in our specific representation (31) and (32), all the variables occurring in (33) and (34) are given in terms of multiplication operators. More generally, all the variables that are affected by the gauge transformations (19) are given in terms of multiplication operators, meaning that the gauge structure of the theory can be carried over to the quantum theory without modification. This is to be compared with the conventional coordinate representation, where the transformation \( \delta \pi^{ik} = -\varepsilon_{i,k} + \eta_{ik} \Delta \xi \) does hardly make sense in the quantum theory. This feature of our specific representation is not a coincidence, and we will come back to this point later on.
The manipulations performed in this section were simple to carry out, because of the linearity of the theory. In particular, the projection operators that are used to perform the orthogonal decomposition into $TT$, $T$ and $V$ parts are constant, and therefore easy to handle. Things are much more involved in non-linear theories, for instance when we have to deal with covariantly transverse components or similar. In the case of non-abelian Yang-Mills theory, we are rather lucky, because the state functional turns out to be already gauge invariant in the coordinate representation (as a result of the linearity of the constraint in the momenta). In General Relativity, as we will show in the next section, this is not the case, and the representation for which the functional is gauge independent is very hard to find.

4 General Relativity

In General Relativity, the first order Lagrangian (in the ADM parameterization) is of the form

$$L = \int \left[ \pi^{ik} \dot{g}_{ik} - N \mathcal{H} - N_i \mathcal{H}^i \right] \, d^3 x,$$

with

$$\mathcal{H} = \frac{1}{\sqrt{g}} (\pi^{ik} \pi_{ik} - \frac{1}{2} \pi^2) - \sqrt{g} R, \quad \mathcal{H}^i = -2 \pi^{ik} \varepsilon_k = 0,$$

where indices are raised and lowered with the spatial metric $g_{ik}$ and its inverse $g^{ik}$, and the semicolon denotes covariant derivation with respect to $g_{ik}$ (note that $\pi^{ik}$ is a tensor density). The formal analysis is identical to that in the previous section. We have the four constraints $\mathcal{H} = \mathcal{H}^i = 0$ and thus consider the four gauge generators

$$G_\varepsilon = \int \varepsilon \mathcal{H} d^3 x, \quad G_\xi = \int \xi^i \mathcal{H}^i d^3 x,$$

which arbitrary parameters $\varepsilon, \xi_i$ (assumed to be such that surface terms can always be omitted). Those generators induce transformations on $\pi^{ik}$ and $g_{ik}$ which can be found by evaluating $\frac{\delta G_\varepsilon}{\delta \pi^{ik}} = \delta_\varepsilon g_{ik}$, $\frac{\delta G_\xi}{\delta g_{ik}} = -\delta_\xi \pi^{ik}$ and similar for $G_\xi$, see [10]. The action of the corresponding pre-quantized operator on the pre-quantized gauge functional $f(g_{ik}, \pi^{ik})$ can be read off from our general result [12].

$$\hat{G}_\varepsilon f = \frac{1}{i} \delta_\varepsilon f - \left( \int \left[ \delta_\varepsilon \pi^{ik} \partial_{ik1} + \delta_\varepsilon g_{ik} \partial^{ik2} \right] d^3 x - G_\varepsilon \right) f$$

$$\hat{G}_\xi f = \frac{1}{i} \delta_\xi f - \left( \int \left[ \delta_\xi \pi^{ik} \partial_{ik1} + \delta_\xi g_{ik} \partial^{ik2} \right] d^3 x - G_\xi \right) f$$

In our previous examples, we used the fact that the constraints were linear (or, more precisely, homogenous of first degree) in certain variables. Here too, this is the case for $G_\xi$, namely we have again $G_\xi = \int (\delta_\xi g_{ik}) \pi^{ik} d^3 x$ just as in the linear theory. Note that an analogue to the relation $G_\varepsilon = -\int (\delta_\varepsilon \pi^{ik}) h_{ik} d^3 x$ of the linear theory does not hold here. In any case, it is easy to see that with the conventional choice $\partial_{ik1} = 0$ and $\partial^{ik2} = \pi^{ik}$ (which leads to $f = \psi(g_{ik})$ in the coordinate polarization), we find $\hat{G}_\xi f = \frac{1}{i} \delta_\xi f$, but $\hat{G}_\varepsilon f \neq \frac{1}{i} \delta_\varepsilon f$. That is, after imposing the constraints, the functional will be invariant under those transformations induced by $\hat{G}_\xi$ but not under those induced by $\hat{G}_\varepsilon$.

The fact that in the coordinate representation, the effect of the constraints $\mathcal{H}^i$ is to render the wave functional invariant under the transformations $\delta_\xi g_{ik}$ and $\delta_\varepsilon \pi^{ik}$ (i.e., under general coordinate transformations in three-dimensional space) is well known, see [7, 8, 9]. On the other hand, the fact that $G_\varepsilon$ has not the effect of rendering
the wave functional invariant under $\delta \varepsilon_{g_{ik}}$ and $\delta \varepsilon_{\pi^{ik}}$ (which correspond, on-shell, to the remaining spacetime diffeomorphisms, see, e.g., [10]) has led to difficulties concerning the interpretation of this constraint, i.e., of the Wheeler-DeWitt equation $H \psi = 0$ (more precisely, $G_{\varepsilon} \psi = 0$). In [7], it is suggested that $H$ should eliminate a further degree of freedom from the theory, but the discussion is transferred to future work. Dirac [8] claims that the meaning of the constraint is that $\psi$ should be independent of deformations of the surface, but this is just what we have proved not to be the case. It is well-established that the Hamiltonian constraint $H \psi = 0$ is not totally understood. A characteristic statement is the following: Roughly speaking, the constraints $\tilde{G}_{\xi} \psi = 0$ and $\tilde{G}_{\varepsilon} \psi = 0$ can be interpreted as requiring the invariance of $\psi$ under the infinitesimal canonical transformations generated by $G_{\varepsilon}$ and $G_{\xi}$, which, as discussed above, correspond to infinitesimal coordinate transformations on the manifold of solutions. For the momentum constraints $\tilde{G}_{\xi} \psi = 0$, this holds literally. [...] It does not appear possible to give as literal an interpretation of the quantum constraint $\tilde{G}_{\varepsilon} \psi = 0$, known as Wheeler-DeWitt equation, as corresponding to the invariance of $\psi$ under a variation of $g_{ik}$ corresponding to an infinitesimal diffeomorphism in spacetime which moves points on $\Sigma$ in the direction orthogonal to $\Sigma$. Nevertheless, this interpretation of the quantum constraints can be viewed as accounting for why $\delta \psi / \delta t = 0$ in the formalism. This statement is taken from an article of Unruh and Wald [10], where for convenience, we have replaced the notation with our own. Further, $\Sigma$ is the three-dimensional manifold, and $\delta \psi / \delta t = 0$ results because the Hamiltonian (on the constraint surface) is zero.

While this is in accordance with our results, the question about the exact interpretation of the Hamiltonian constraint remains. On the other hand, it is clear that if one would use a representation in which the constraints really imply gauge invariance of $\psi$, then the problem would be trivially solved. How this is to be achieved is clear from the corresponding procedure in the linear theory. Namely, instead of taking $\vartheta_{ik1} = 0$ and $\vartheta_{ik2} = \pi^{ik}$ (coordinate representation), we have to modify this in a way not to destroy the already obtained invariance under $G_{\xi}$. This is done by recognizing that not all components of $\vartheta_{ik2}$ are actually contained in the term $f \delta \xi_{g_{ik}} \vartheta_{ik2}$ in (39). We can thus take some components and shift them over (in terms of the canonically conjugated variables) to $\vartheta_{ik1}$, which results in some components being brought into the momentum representation. Also, some components of $g_{ik}$ (and the conjugate components of $\pi^{ik}$) do not appear at all in (39) and (39), as was the case with $\tau \pi_{i1}$ and $\tau \pi_{i2}$ in the linear theory. For those, we have again the choice of using a coordinate of momentum representation, without the transformation properties of $f$ (and thus of $\psi$) being affected.

Although this sounds all very nice, it is obvious that we cannot perform this explicitly in the full theory. Because, if we did, we would have identified the dynamical variables, and since those satisfy trivial equations of motion ($H = 0$), we would have solved the Einstein equations completely. In other words, the above procedure is in fact of the same degree of difficulty than solving the Einstein equations, or, on the quantum level, solving the Wheeler-DeWitt equation. There is no magic way around the non-linearities of General Relativity. What one can do, however, is to check for specific representations, whether the corresponding functional is gauge invariant or not. As outlined above, this is not the case for the coordinate representation, and it is also not hard to show that the same holds true for a pure momentum representation.

Our approach can nevertheless be useful for the interpretation of the Wheeler-DeWitt equation in another way. Namely, there is a tendency in the literature to relate any kind of difficulties one encounters during the analysis of General Relativity directly to the specific features of generally covariant theories. Since there are indeed certain features that one does not encounter in conventional theories, it would be wise to carefully isolate them from possible additional problems, that are not related, e.g., to the reparameterization invariance. In this sense, if one wishes to correctly interpret the Wheeler-DeWitt equation, a good starting point is to have a
general idea of what could be the answer to the following questions: What does it mean that a wave functional is not gauge independent after the constraints have been imposed? And a directly related question: What is the meaning of a constraint if it is not to eliminate unphysical degrees of freedom from the wave functional and thus to render it invariant under the transformation induced by the same constraint on the phase space variables? Obviously, those are questions that are completely unrelated to the more specific problems of General Relativity concerning, e.g., the problem of time, despite the connection there might be between the later issue and the Hamiltonian constraint. It concerns, e.g., the fourth constraint of the linear spin-two theory in the coordinate representation, but also electrodynamics and Yang-Mills theories in the momentum representation.

In section 5 we will present simple models, for which it is possible to identify explicitly the representation(s) in which the constraints eliminate the gauge degrees of freedom from the state functional. As in the linear spin-two theory, they turn out to be mixed representations. Before, in section 5, we briefly analyze the case of a relativistic point-particle.

5 Relativistic point-particle

The special relativistic point-particle is described by the Lagrangian

$$L = -m\sqrt{x^\mu x^\nu} \ (\mu = 0, 1, 2, 3)$$

or, in first order form,

$$L = p_\mu \dot{x}^\mu - \lambda (p_\mu p^\mu - m^2).$$

(40)

Note that we use the notation $x^0$ for the time coordinate, and $\dot{t}$ for the parameter of the theory, i.e., $\dot{x}^\mu = \frac{dx^\mu}{dt}$. The Lagrange multipliers $\lambda$ is arbitrary and leads to the constraint $p_\mu p^\mu - m^2 = 0$, which generates the transformations $\delta x^\mu = \varepsilon^\mu_{\ \pi}$ and $\delta p_\mu = 0$. The constraint can be solved for $p_0$ (assumed to be positive), leading directly to the reduced dynamics in terms of three canonical pairs of variables. Here, instead, we wish to perform the quantization first and then impose the constraint on the quantum states of the theory. Note that the Hamiltonian itself is zero, and therefore, the Schrödinger equation leads to $\partial \psi/\partial t = 0$. The dynamics, therefore, is obtained from the constraint alone, which leads, in the coordinate representation, to the Klein-Gordon equation. However, since the constraint is not homogenous of first degree in the momenta, it is immediately obvious from (12) that in that representation (obtained again from $\vartheta_{\mu\nu} = 0$ and $\vartheta_{\mu 2} = p^\mu$), the wave function will not be gauge invariant, i.e., the Klein-Gordon equation does not remove the unphysical degrees of freedom from the theory. (In fact, it does not even make sense to ask the question whether a certain function $\psi(x^\mu)$ is invariant under the transformation $\delta x^\mu = \varepsilon^\mu_{\ \pi}$, since $p^\mu$ is supposed to be represented by a differentiation operator. Since classically, we have $p^\mu = \text{const}$ (on-shell), one could think of considering transformations of the form $\delta x^\mu = \varepsilon a^\mu$ with constant $a^\mu$ instead. It is not hard to show for explicit solutions of the Klein-Gordon equation that $\psi$ will not be invariant under such transformations neither.)

This short-come is readily fixed by linearizing the constraint via the introduction of a new variable $P_0 = p_\mu p^\mu - m^2$ and its conjugate $X^0 = \frac{1}{2} \frac{x^0}{p_0}$. Altogether, we perform the phase-space transformation

$$X^0 = \frac{1}{2} \frac{x^0}{p_0}, \quad X^i = x^i - \frac{p^i x^0}{p_0}, \quad P_0 = p_\mu p^\mu - m^2, \quad P_i = p_i,$$

(41)

which is easily shown to represent a canonical transformation, either by checking the canonical Poisson brackets or by noting that $p_\mu \dot{x}^\mu = P_\mu \dot{X}^\mu$ (up to a total derivative). The first order Lagrangian now takes the simple form $(i = 1, 2, 3)$

$$L = P_i \dot{X}^i - \lambda P_0,$$

(42)

where in the kinetic term, the constraint $P_0 = 0$ can be used, since $P_0$ is coupled with an arbitrary multiplier anyway. The constraint being linear in $P_0$, it is obvious that we have to put $X^0$ into the coordinate representation
in order to obtain a gauge invariant wave function. Note that the only gauge variable is now $X^0$, transforming as $\delta X^0 = \varepsilon$. The remaining variables $(X^i, P_i)$ are physical and we can use any representation we wish. If we choose the coordinate representation, we have $\psi = \psi(X^i, X^0)$, and the constraint $P_0 \psi = \frac{1}{\sqrt{\epsilon}} \frac{\partial}{\partial X^0} \psi = 0$ leads to $\psi = \psi(X^i)$, which is gauge invariant and coincides with the result obtained by the explicit reduction of the theory. Although this appears now in the form of a pure coordinate representation, in terms of the initial variables, it is actually a mixed representation. Namely, one has to use a functional depending on certain combinations of the phase-space variables, $\psi = \psi(x^0/p_0, x^i - p^i x^0/p_0)$, and then consider the following operators

$$\dot{x}^i = x^i - \frac{x^0}{p_0} (p^i - \frac{1}{i} \frac{\partial}{\partial x^0})$$

$$\dot{p}_0 = \sqrt{\frac{2}{i} \frac{\partial}{\partial (x^0/p_0)} + \frac{\partial^2}{\partial (x^i - p^i x^0/p_0) \partial (x^i - p^i x^0/p_0)} + m^2}$$

The constraint $(\dot{p}_i \dot{p}^i - m^2) \psi = 0$ then implies that $\psi$ does not depend on $x^0/p_0$, and the resulting wave function $\psi(x^i - p^i x^0/p_0)$ is indeed gauge invariant. As one can see, we are actually quite polite using the mild expression **mixed representation** for the above.

It is further interesting to observe that the constraint equation in the new variables, $\frac{\partial}{\partial x^0} \psi = 0$, cannot be obtained (e.g., with $X^0$ as time variable) from a Lagrangian (at least not without the help of auxiliary fields), quite in contrast to the Klein-Gordon equation. In particular therefore, we do not have a canonical way to perform a second quantization, i.e., to treat $\psi$ as a quantum operator.

In relation to General Relativity, if we ask questions about the interpretation of the Wheeler-DeWitt equation, we should first answer the corresponding questions on the interpretation of the Klein-Gordon equation. Apart from the fact that it describes (in the coordinate representation) the dynamics of the system, we would like to know its relation to the symmetry transformations and to the elimination of the unphysical degrees of freedom. All we can give here is a negative statement: The Klein-Gordon equation does not remove the gauge degrees of freedom from the wave function. On the other hand, in the new representation, the interpretation of the constraint equation is completely clear. It removes the gauge variable from the wave function, which is also all the dynamics we get. For the rest, the explicit form of $\psi$ has to be determined by physical arguments (boundary conditions).

## 6 Cosmological models

First, we consider homogenous spacetimes with metric

$$ds^2 = N^2 dt^2 - R^2 (\exp(2b_1)dx^2 + \exp(2b_2)dy^2 + \exp(-2b_1 - 2b_2)dz^2),$$

depending on 4 variables $N(t), R(t), b_1(t)$ and $b_2(t)$. The corresponding vacuum Einstein field equations are derived from

$$L = \frac{1}{N} [-2R^i \dot{b}_i + \dot{b}_1 + \dot{b}_2] + 6R \dot{R}^2].$$

Such models have been studied in [11] where the detailed analysis can be found. It is convenient to perform a change of variables, defining

$$\tilde{N} = \frac{N}{2} \exp(-\sqrt{3}X), \quad X = \sqrt{3} \ln R.$$
This leads to \( L = \frac{1}{2}\left(-\left(\dot{b}_1^2 + \dot{b}_1 \dot{b}_2 + \dot{b}_2^2\right) + \dot{X}^2\right) \) and to the first order Lagrangian

\[
L = \pi \dot{X} + p_1 \dot{b}_1 + p_2 \dot{b}_2 - \dot{N} \left[ \frac{\pi^2}{4} - \frac{1}{3}(p_1^2 + p_2^2 - p_1 p_2) \right],
\]

where \( \pi, p_1 \) and \( p_2 \) are the momenta conjugated to \( X, b_1 \) and \( b_2 \), respectively. One can directly solve the constraint for \( \pi \) and derive the reduced Lagrangian. Here instead, we are interested again in imposing the constraint on the quantum states. Since the constraint is not homogeneous of first degree in neither variable, we perform a canonical transformation

\[
B_1 = b_1 + \frac{4}{3} \frac{p_1 - \frac{1}{2} p_2}{\pi} X, \quad B_2 = b_2 + \frac{4}{3} \frac{p_2 - \frac{1}{2} p_1}{\pi} X,
\]

\[
Y = \frac{2 \pi}{\sqrt{3}}, \quad \Pi = \frac{\pi^2}{4} - \frac{1}{3}(p_1^2 + p_2^2 - p_1 p_2),
\]

with \( p_1 \) and \( p_2 \) as before. We now find

\[
L = p_1 \dot{B}_1 + p_2 \dot{B}_2 + \Pi \dot{Y} - \dot{N} \Pi.
\]

The fact that the kinetic terms are still in canonical form (and thus the symplectic two-form is unchanged) proves that the above transformation was indeed canonical. The constraint \( \Pi = 0 \) induces the gauge transformation

\[
\delta Y = \epsilon, \quad \delta \pi = \epsilon \pi,
\]

where \( \epsilon \) is a gauge parameter. Since the constraint is linear in \( \Pi \), a gauge invariant wave functional is obtained by choosing a coordinate representation for \( Y, \pi \), i.e., \( \dot{Y} = Y \) and \( \dot{\Pi} = \frac{4}{3} \delta Y \). The variables \( B_1 \) and \( B_2 \) are physical and can be taken in any representation. They represent the two dynamical degrees of freedom of the (homogenous) gravitational field. In particular, in the coordinate representation, we have \( \psi = \psi(B_1, B_2, Y) \), and the constraint imposed on \( \psi \) eliminates the gauge variable \( Y \), i.e., \( \psi = \psi(B_1, B_2) \), which is trivially gauge invariant and is identical to the results one obtains by direct elimination of \( \Pi \) from the classical theory (reduction). Similar as in the case of the point-particle, the representation, when expressed in terms of the initial variables, is far from being a pure coordinate representation. We also note that from (49), we find the equation of motion \( \ddot{N} - \dot{Y} = 0 \), which determines \( \dot{N} \). The equation is gauge invariant, and we observe further that \( \dot{N} \) (and thus also \( N \), see (45) and (48)) is given, in the specific representation, in terms of simple multiplication operators.

As a further example, we consider flat Robertson-Walker spacetimes, \( ds^2 = N(t)^2 dt^2 - R(t)^2 \delta_{ik} dx^i dx^k \), with a minimally coupled massless scalar field \( \varphi(t) \). The Lagrangian is here (see (12, 13)) \( L = -\frac{\dot{R}^2}{N} + \frac{\dot{R}^2}{2N} \frac{\varphi^2}{R^2} \), which leads to the first order Lagrangian \( L = \pi_R \dot{R} + \pi_\varphi \dot{\varphi} + N(\frac{\pi_{\varphi}^2}{2N} - \frac{\pi_\varphi^2}{2R^2}) \). Performing a change of variables \( X = \varphi - \sqrt{2}\ln R, \quad Y = \varphi + \sqrt{2}\ln R \) and \( \dot{N} = 2R^{-3}N \) in the second order Lagrangian, we obtain the simplified first order form

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

with constraint \( \pi_X \pi_Y = 0 \), which, in contrast to the initial form, is free of ordering problems. The induced transformations are \( \delta X = \varepsilon \pi_Y, \quad \delta Y = \varepsilon \pi_X \) and \( \delta \pi_X = \delta \pi_Y = 0 \). The Lagrangian is invariant if \( \delta \dot{N} = \dot{\varepsilon} \). Classically, we can solve the constraint by \( \pi_X = 0 \) or by \( \pi_Y = 0 \), resulting in \( \delta Y = 0 \) or \( \delta X = 0 \). Thus, depending on the set of classical solutions one refers to, the dynamical variables are either the pair \( (X, \pi_X) \), or the pair \( (Y, \pi_Y) \). On the other hand, the Wheeler-DeWitt equation, in the conventional coordinate representation, leads to \( \frac{\delta^2}{\delta X \delta Y} \psi(X, Y) = 0 \), i.e., \( \psi = \psi_1(X) + \psi_2(Y) \), which is not gauge invariant in neither case. We conclude that the Wheeler-DeWitt equation does not eliminate the unphysical degrees of freedom from the state functional.
This is consistent with the general relation \([12]\) and the fact that the constraint is not of first degree in the momenta.

On the other hand, the constraint is linear in each momentum \(\pi_X\) and \(\pi_Y\) separately. Therefore, if we choose a mixed representation with either \(X\) or \(Y\) in the momentum representation, the resulting wave functional should be gauge invariant. Let us therefore adopt the following representation

\[
\hat{X} = -\frac{1}{i} \frac{\partial}{\partial \pi_X}, \quad \hat{\pi}_X = \pi_X, \quad \hat{Y} = Y, \quad \hat{\pi}_Y = \frac{1}{i} \frac{\partial}{\partial Y}.
\]

and \(\psi = \psi(\pi_X, Y)\). The constraint equation now reads \((\pi_X \frac{\partial}{\partial X}) \psi(\pi_X, Y) = 0\). There are two cases to consider. First, if \(\pi_X\) is different form zero, then the solution of the constraint is \(\psi = \psi(\pi_X)\) which is gauge invariant in view of \(\delta \pi_X = 0\). On the other hand, if \(\pi_X = 0\), then there is no condition on \(\psi\), which is therefore a general function of \(Y\), \(\psi = \psi(Y)\). This too is gauge invariant, since \(\delta Y = -\pi_X = 0\). Nevertheless, we would rather consider this as a condition on \(\pi_X\) and not on \(\psi\) (similar to the constraint \(\Delta^R h \psi = 0\) in the spin-two theory) and conclude that in this case, we are not using the appropriate representation. We then choose instead the representation with the roles of \(X\) and \(Y\) interchanged and end up with \(\psi = \psi(\pi_Y)\). The fact that we have to distinguish between two cases is typical for General Relativity, where the dynamical variables cannot be determined in a general form (e.g., in terms of traceless-transverse components of \(g_{ik}\) or similar), but depend on the specific form of the corresponding classical solutions. This is already obvious from the fact that the constraint \(\pi_X \pi_Y = 0\) has two sets of classical solutions. See also the discussion in \([6]\).

Thus, once again, a mixed momentum/coordinate representation is needed in order for the constraint to do what it is expected to do, namely to eliminate the unphysical degrees of freedom from the theory. It is not hard to verify that \((51)\) corresponds to a mixed representation also in the initial variables \(R, \pi_R, \varphi, \pi_\varphi\).

We also note that from \((50)\), we find the gauge invariant equations \(\hat{X} + \hat{N} \pi_Y = 0\) and \(\hat{Y} + \hat{N} \pi_X = 0\). Thus, if \(\pi_X \neq 0\), we can express \(\hat{N}\) in terms of the multiplication operator \(Y\), while in the other case, we take again the second representation and express \(\hat{N}\) in terms of the multiplication operator \(X\). On the other hand, in the conventional coordinate representation (Wheeler-DeWitt approach), \(\hat{N}\) is represented by a differentiation operator, see \([6]\).

### 7 Discussion

The method for obtaining a gauge invariant state functional is now clear. It consists simply in using a representation where the gauge variables are represented by multiplication operators, and the corresponding, canonically conjugated constrained variables by differentiation operators. In that way, the state functional will depend on the gauge variables, which are then eliminated by the action of the constraints. For the physical variables, there is no restriction, and we have a complete symmetry between momentum and coordinate representation. The geometric quantization formalism presented in section \([2]\) is simply a justification for this simple recipe, which one might or might not find useful.

There remains the question of the meaning of the constraints when we use a representation different from the above. Consider, for instance, the forth constraint of the spin-two theory, \(\Delta^R h = 0\). If we use a pure coordinate representation, \(\psi = \psi(T^R h_{ik}, h_i, \gamma h)\), then the remaining three constraints eliminate the gauge variable \(h_i\). Thus, we are left with \(\psi = \psi(T^R h_{ik}, \gamma h)\). But this is already gauge invariant. This shows once again that the effect of the fourth constraint cannot be to render \(\psi\) gauge invariant. Instead, we have argued that the equation \(\Delta^R \psi(T^R h_{ik}, \gamma h) = 0\) (suppressing the integration and the gauge parameter for simplicity) is actually not a condition on \(\psi\), but rather on \(\gamma h\), and leads to \(\Delta^R h = 0\) (or \(\gamma h = 0\)). Since this is rather an explicit elimination (reduction) of variables via a classical equation of motion than the solution to a quantum constraint equation,
we considered this to be outside of the spirit of the original Dirac method. There is, however, a different interpretation to the above equation, which is adopted, e.g., in [2], namely $\Delta^2 \psi (\tau^2 \hbar_{ik}, \hbar) = 0$ is to be solved by functionals $\psi$ with support only on configurations with $\Delta^2 \hbar = 0$ (or $\hbar = 0$). While physically, this leads to the same results, from a mathematical standpoint, it is a quite different statement than merely requiring $\Delta^2 \hbar = 0$, since it is indeed a condition on $\psi$ now. Nevertheless, we are still not completely happy with such an interpretation, because it does not really render $\psi$ independent of $\hbar$ (as is the case in the mixed representation). Since, if $\psi$ were independent of $\hbar$, there would obviously be no need to differentiate between $\hbar \neq 0$ and $\hbar = 0$.

The functional still depends implicitly (via the definition of the support) on $\hbar$. A similar situation holds in electrodynamics, if we use a pure momentum representation, $\psi = \psi(E)$. Also here, the functional is already gauge invariant (since $\delta E^i = 0$), and one can interpret the constraint $E^i \psi = 0$ by requiring that $\psi$ has support only on the transverse part of $E^i$.

While the above interpretation works quite well and differs only esthetically from the corresponding approach with mixed representations (after all, we are not really interested in the gauge dependent parts anyway, so any way of eliminating them should be equally acceptable), the situation is different for more complicated theories. Consider non-abelian Yang-Mills theory in a pure momentum representation, with $\psi = \psi(E)$.

Recall that the constraint reads $G = \int d^3 x \varepsilon^{a}(\partial_i E^a_i + f_{ab}^c A^b_i E^c_i)$. But now, the equation $\hat{G} \psi(E)$ cannot be interpreted as "$\psi(E)$ has support only on configurations with $\partial_i E^a_i + f_{ab}^c A^b_i E^c_i = 0$", since the latter expression contains the operator $A^a_i = -\frac{1}{\hbar} \frac{\delta}{\delta E^a_i}$.

An idea is to treat the above partly as a condition on the support of $\psi$ (as in electrodynamics) and partly as differential equation. Namely, we first imply the second term of the constraint on $\psi$, in the form $\int d^3 x \varepsilon^{a} f_{ab}^c E^c_i \delta E^a_i \psi(E) = 0$. It is not hard to show that this requires $\psi(E)$ to be gauge invariant (since $E^a_i$ transforms covariantly, i.e., as a vector). In addition, we interpret the remaining term of the constraint as in electrodynamics, namely that $\psi(E)$ has only support on the transverse part of $E^i$ (i.e., on $E^i_a$ satisfying $E^a_i = 0$). In this way, we end up with gauge invariant functionals $\psi(E)$, e.g., $\psi = \psi(E) E^a_k \psi^k$. The only thing we have to worry about is whether we have possibly imposed too many conditions on $\psi$, because it seems to be a stronger requirement for each term of the constraint separately to annihilate $\psi$ than merely to impose the constraint. This is true (since we have already shown that $\hat{G} \psi = 0$ alone does not lead to a gauge invariant $\psi$), but it is not physically relevant. The gauge dependent parts of $\psi$ are unphysical anyway, so rendering $\psi$ gauge invariant cannot do any harm. Once this has been done, the remaining condition $E^a_i \psi = 0$ is a direct consequence. So, in a sense, we have done more than the constraint requires, but this concerns only unphysical contributions in $\psi$.

Note that the above argumentation is not unsimilar to the approach adopted in [1] and [2], where a gauge dependent factor is extracted from the wave functional, leading to a functional that is annihilated by the rotational part of the constraint generator. On the other hand, it is hard to imagine how a similar argumentation could be applied in the case of the Wheeler-DeWitt equation. (Also, it fails completely in the case of the point-particle in the coordinate representation.)

Let us compare the above with the approach presented in section [2], which is based on the use of a gauge invariant functional. Being interested in a momentum representation, we should, at least, put the dynamical variables into the momentum representation. Even though we do not know exactly which are the physical (gauge invariant) components of $A^a_i$, we can recognize that the transverse components $\tau^a_i$ transform covariantly (i.e., as vectors). (This holds actually only for infinitesimal transformations, see below.) Therefore, let us choose $\partial_{a_2}^i = E^i_a$ and $\partial_{a_1}^i = -\tau^a_i$. (Our notation is $B_i = \tau_i B_i + \tau_i B_i$, with $\tau_i B_i = \frac{\delta}{\delta \lambda} B_k$.) From [12], we find that $\hat{G} = \frac{1}{\hbar} \delta f$, as required. We use the polarization $\tau^a_{a_2} = 0$ and $\tau^a_{a_1} = 0$, leading to $\delta f/\delta \tau^a = 0$ and $\delta f/\delta E = 0$,
i.e., to \( f = \psi(\mathfrak{t}A, \mathfrak{t}E) \). The constraint now leads to
\[
\hat{G}\psi = \frac{1}{i} \int d^3x \left( \frac{\delta \psi}{\delta \mathfrak{t}A^i} (-\varepsilon^a_i - f_{db}^a \mathfrak{t}A^b \varepsilon^d) - \frac{\delta \psi}{\delta E_a^c} f_{da}^c \mathfrak{t}E_a^c \varepsilon^d \right) = 0,
\]
which results in \( \delta \psi / \delta \mathfrak{t}A^i = 0 \) and \( \int d^3x \frac{\delta \psi}{\delta E_a^c} f_{da}^c \mathfrak{t}E_a^c = 0 \). The second relation is again recognized as the invariance of \( \psi(\mathfrak{t}E_a) \) under rotations, and thus, we find the same results as before. Thus, if we start directly from a gauge invariant pre-quantized functional \( f \), there is not need to split the constraint into two terms or to extract a gauge dependent phase from the functional. One is directly led to a consistent momentum representation.

We conclude that, although in certain cases, it is possible to interpret constraints which contain variables in form of multiplication operators as a condition on the support of the wave functional, such a procedure is, on one hand, not really elegant, because it means that implicitly the wave functional depends nevertheless on those variables, and on the other hand, it leads to additional difficulties in more complex cases, where one has to interpret a part of the constraint as differential equation and another part as condition on the support. In other cases, for instance the relativistic point-particle in the coordinate representation, there does not seem to exist a similar way to interpret the constraint. It is therefore more systematic and more straightforward to choose a representation that eliminates all unphysical fields from the wave functional directly by true differential equations.

We should note, however, that the above argumentation was based on infinitesimal gauge transformations and does not take account of the problems related to the Gribov ambiguity. In fact, it is not completely accurate to consider \( \varepsilon^a \) and \( \varepsilon^a_i \), in (52) as independent. There are functionals that depend on \( \mathfrak{t}A^i \) and for which the above \( \hat{G}\psi \) is zero nevertheless. For instance, we can take \( \psi = \int F_{\mathfrak{t}ik}^a (\mathfrak{t}A) F_{\mathfrak{t}a}^{ik} (\mathfrak{t}A) d^3x \), where \( F_{\mathfrak{t}ik}^a (\mathfrak{t}A) \) is the Yang-Mills tensor with \( \mathfrak{t}A^i = 0 \). This leads to \( \hat{G}\psi = 0 \), because we have \( \delta \psi / \delta \mathfrak{t}A^i \sim D_i F^{ik} \) and \( D_i D_k F^{ik} = 0 \), where both \( F \) and the covariant derivative \( D \) are formed with \( \mathfrak{t}A^i = 0 \). This is related to the fact that \( \mathfrak{t}A^i \) and \( E_a^c \) do not describe the theory completely, since, e.g., if \( E_a^c = \mathfrak{t}A^a \), the gauge invariant quantity \( F_{\mathfrak{t}ik}^a F^{ik} \) can still be different from zero, and can be further traced back to the fact that the decomposition \( A = \mathfrak{t}A^i + \mathfrak{t}A \) is not gauge invariant. Therefore, the gauge invariant representations do not replace the detailed analysis carried out, e.g., in \([13]\), concerning the identification of the physical variables, but they could nevertheless provide an alternative starting point which deserves further study.

As to General Relativity, it represents a special case. As we have mentioned before, here the dynamical variables cannot be specified in a general form. This is a matter of principle, and not a result of us being unable to solve the corresponding equations. This means in particular that we cannot represent the gauge variables by multiplication operators and the constrained variables by differentiating operators without specifying a specific set of classical solutions we refer to. We have encountered this feature in our second example in section [6] where two different representations had to be used, according to whether \( (X, \pi_X) \) or \( (Y, \pi_Y) \) are the physical variables. This is completely similar to the problems one faces during the explicit reduction of the theory, where one has to solve the classical equation \( \pi_X \pi_Y = 0 \) either by \( \pi_X = 0 \) or by \( \pi_Y = 0 \), see [8], or the corresponding problems that arise when one decides to fix the gauge explicitly (choice of time coordinate), which has to be done by \( X = f(t) \) in one case, and by \( Y = f(t) \) in the other. One could see in this an advantage of the conventional Wheeler-DeWitt approach (coordinate representation), where this question is left open. There, we have solutions \( \psi(X,Y) = \psi_1(X) + \psi_2(Y) \) and we do not need to decide whether \( X \) or \( Y \) is the physical variable. While this seems reasonable from the point of view that the quantum theory should not directly refer to a specific set of classical configurations (e.g., \( \pi_X = 0 \) or \( \pi_Y = 0 \)), it is nevertheless also clear that sooner or later, one has to remove the gauge dependent parts from \( \psi(X,Y) \). Whether one does this directly as conditions
on $\psi$ or via boundary conditions or by an appropriate construction of the scalar product, it does not really change the fact that, in order to remove them, one will first have to decide which degrees are physical and which are not. In any case, we retain the fact that, while the exact meaning of the Wheeler-DeWitt equation in the coordinate representation is unclear [10], our analysis shows that there are representations for which there is no doubt whatsoever on the physical interpretation of the constraint.

There is one more important feature of the gauge invariant representations. As we have mentioned at the end of section [3] in the spin-two theory, we found that the Lagrange multipliers $h_{00}$ and $h_{0i}$ could be expressed in terms of multiplication operators. The same was shown for $N$ (or $\dot{N}$) in our cosmological examples, section [6] and it is not hard to argue that this will be the case for Lagrange multipliers in general, whenever we use our specific representations. (That results because, for the wave functional to become gauge invariant, the constraints the multipliers apply to must be homogenous of first degree in the variables which are represented by differentiation operators.) While this is in most cases not of interest, since the multipliers are unphysical anyway, we have shown in [9] that the situation is different in the linear spin-two theory and in General Relativity. Namely, while in conventional theories, the configuration can be completely specified by the constrained variables and the dynamical variables alone, in the latter cases, there are physical (i.e., invariant) quantities that cannot be expressed without the help of the multipliers. This concerns for instance the (four dimensional) scalar curvature in General Relativity which contains $N$. More specifically, the equations (43) and (44) in the spin-two theory as well as equation $\dot{N} - \dot{Y} = 0$ in our first example in section [6] and the equations $X + N\pi_Y = 0$ and $Y + N\pi_X = 0$ in the second example of the same section are all gauge invariant. (In the latter case, only one of both will determine $\dot{N}$, according to whether $\pi_X = 0$ or $\pi_Y = 0$.) It is clear, at least on the classical level, that one cannot do without those equations, since if they are omitted, this means that even after the gauge is fixed, there remains one undetermined invariant expression in the theory. More explicitly, in a Lagrangian of type (49), we would usually omit the third term, arguing that $\Pi$ is coupled with an arbitrary multiplier anyway (fourth term), just as we did in (42) with the term $P_0X^0$. This, however, would lead to $\dot{N} = 0$ (and thus $N = 0$), which is obviously unacceptable.

On the other hand, the equations for the multipliers $N, N_i, h_{00}, \ldots$ can only be obtained by classical means, namely by variation of the Lagrangian before the constraints are solved. Thus, such equations are neither quantum constraints to be imposed on the states, nor are they obtained, e.g., in the form of Heisenberg equations, as are the dynamical equations. In fact, they are irrelevant for the quantum dynamical evolution of the system and do not appear, e.g., in the Schroedinger equation. Thus, as has been outlined in [9], they simply represent operator relations, that is, $N, N_i, h_{00}, \ldots$ are given in terms of the remaining operators. (Although irrelevant for the true quantum dynamics, they can still not be omitted, since after all, the quantum theory should also contain the classical limit.) Thus, we have the rather strange situation that we have quantum operators that can only be determined by a classical variation. In the conventional, pure coordinate representation, it turns out that $h_{00}, h_{0i}$, as well as $N$ in cosmological models [11] are given in terms of differentiation operators (and their inverse). Using the invariant representations instead, they are all given in terms of simple multiplication operators. In other words, they can be treated as classical functions. This seems much more appropriate for a quantity that has to be determined classically from a Lagrangian, and we consider this an additional advantage of the specific representations. Possibly, this observation could also be useful in the reversed direction, namely for the determination of the invariant representations. That is, instead of analyzing directly the constraints, one could analyze the field equations for $N$ and $N_i$ and choose the representation such that $N$ and $N_i$ are given in terms of classical functions.

Moreover, the fact that both the gauge variables as well as the multipliers are represented by multiplication operators in our specific representations allow us to carry over the gauge structure of the theory directly to the quantum case without modification. As mentioned before, e.g., the transformation $\delta \pi_{ik} = \varepsilon_{i,k} + \eta_{ik}\Delta \varepsilon$ would be hard to interpret in the quantum theory if we use a pure coordinate representation. As is easily
checked, we encounter the same situation in our remaining examples. In this sense, the use of our specific representations combines both the features of the Hamiltonian reduction method (Faddeev-Jackiw), where only the dynamical degrees of freedom are quantized right from the start, and the conventional Dirac procedure, where we quantize the complete set of canonical variables and impose the constraints on the physical states. Namely, although we follow the Dirac procedure, at the end, the Lagrange multipliers and the gauge variables are given by multiplication operators anyway, just as if they had not been quantized at all.

8 Summary

It is conventionally assumed that the constraints arising in gauge theories play, in the quantum theory, the role of eliminating the unphysical degrees of freedom from the state functional. We have shown in this article that for this to hold, one has to use very specific operator representations. Performing an analysis based on the approach of geometric quantization, it was shown that for the constraints to render the state functional gauge invariant, the constrained variables have to be represented by differentiation operators, while the corresponding canonically conjugated gauge variables are to be represented by multiplication operators. No restriction exists for the representation of the physical (dynamical) variables.

The conventional coordinate representation of electrodynamics and non-abelian Yang-Mills theory satisfy the above requirements, but not, e.g., the pure momentum representation. On the other hand, in the linear spin-two theory and in General Relativity, the coordinate representation is easily shown not to be of the required form. This results, e.g., in the fact that the Wheeler-DeWitt equation does not render the wave functional gauge invariant under variations of the metric that correspond to infinitesimal diffeomorphisms orthogonal to the three-dimensional space manifold. In the linear theory, it is readily shown that gauge invariance of the functional can only be achieved with representations where certain components of $h_{ik}$ are represented by multiplication operators, and others by differentiation operators, i.e., with mixed momentum/coordinate representations. In General Relativity, the corresponding representations cannot be found in general, but we have obtained similar results for simple cosmological mini-superspace models. In contrast to the Wheeler-DeWitt equation in the conventional coordinate representation, whose physical meaning in relation to the elimination of unphysical degrees of freedom is unclear, in the new, mixed representations, the interpretation is straightforward, since the constraint now explicitly removes the gauge variables from the state functional, leaving us with the physical, gauge invariant functional.

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