Modified Ostrogradski formulation of field theory

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Abstract

We present a method for the Hamiltonian formulation of field theories that are based on Lagrangians containing second derivatives. The new feature of our formalism is that all four partial derivatives of the field variables are initially considered as independent fields, in contrast to the conventional Ostrogradski method, where only the velocity is turned into an independent field variable. The consistency of the formalism is demonstrated by simple unconstrained and constrained second order scalar field theories. Its application to General Relativity is briefly outlined.

1 Introduction

There are two main properties one usually requires a Hamiltonian to possess. First, it should be a conserved quantity, the energy, and second, it should generate the time evolution of the system under consideration. Both features are intimately related, since in relativistic theories, the energy can be viewed as the variable canonically conjugate to time. However, since the Hamiltonian formalism is based on a 3+1 split of spacetime, this relation is not always directly obvious. As a matter of fact, in classical mechanics, but also in field theory, the Hamiltonian is usually introduced via a Legendre transformation of the Lagrangian, and the relation to the energy (i.e., to the time component of the integrated stress-energy tensor, in the field theory case) is only established afterwards and appears rather as a coincidence.

Here instead, we choose to proceed the other way around, that is, we start from the expression for the energy and try to find a set of canonical phase space variables such that the Hamiltonian that emerges after substitution of those variables into the initial expression, does indeed generate the time evolution of the system.

The stress-energy tensor for second order theories can be derived with Noether’s theorem (see our review paper [2]) from invariance of the theory under coordinate transformations. Assume that the fields, collectively denoted with \( \varphi \), transform as

\[
\delta \varphi = \xi^i \varphi_{,i} + \frac{1}{2} \xi^i_{,k} (\sigma \varphi)^k_{,i},
\]

where \((\sigma \varphi)^k_{,i}\) denotes the action of the generators of the general linear group on \( \varphi \). The explicit form depends on the scalar, vector or tensor nature of the fields \( \varphi \). (In other words, \( \delta \varphi \) is the Lie derivative of the field with respect to \( \xi^i_{,i} \).) Invariance under global transformations \( \xi^i = const \) leads to \( \tau^k_{,i,k} = 0 \), where the canonical stress-energy tensor is defined as

\[
\tau^k_{,i} = \left[ \frac{\partial L}{\partial \varphi_{,k}} - \left( \frac{\partial L}{\partial \varphi_{,k,l}} \right)_{,l} \right] \varphi_{,i} + \frac{\partial L}{\partial \varphi_{,k,l}} \varphi_{,i,l} - \delta^k_i L.
\]
It can further be shown (see [1] or [2]) that for generally covariant Lagrangians, \( \tau^k_i \) can be brought into the form

\[
\tau^k_i = \left[ -\frac{\partial L}{\partial \dot{\varphi}_{k,i}} \varphi - \frac{1}{2} \frac{\partial L}{\partial \dot{\varphi}_i} (\sigma \varphi)^k_1 - \frac{1}{2} \frac{\partial L}{\partial \dot{\varphi}_i, l} \left[ (\sigma \varphi)^k_1 \right]_l \right] + \frac{1}{2} \left[ \frac{\partial L}{\partial \varphi_{i,m,l}} (\sigma \varphi)^k_1 \right]_{m,l},
\]

where the expression in the first bracket was shown to be antisymmetric in \( kl \), and the totally symmetric part (in \( mlk \)) of the expression in the second bracket was shown to be zero. As a result, \( \tau^k_{i,k} = 0 \) identically, in accordance with the second Noether theorem.

In first order theories, it is convenient to introduce four momentum variables \( \pi^{(i)} = \partial L / \partial \dot{\varphi}_{i} \), and then perform the 3+1 split with the help of a timelike unit vector \( n^i \), which specifies the direction of the time evolution. The physical momentum is then given by \( \pi = \pi^{(i)} n_i \) (and the velocities by \( \dot{\varphi}_i n^i \)). In this way, one can set up an explicitly covariant Hamiltonian formulation of the theory (see [3]). Throughout this paper, we assume \( n_i = \delta^0_i \), such that \( \pi = \pi^{(0)} \). The introduction of \( \pi^{(i)} \) is nevertheless useful, since it allows to write the stress-energy tensor in the simple form \( \pi^{(k)} \varphi_i - \delta^k_i L \).

Based on those considerations, it is natural, in the framework of second order theories, to introduce the following momenta

\[
\pi^{(i)} = \frac{\partial L}{\partial \dot{\varphi}_i}, \quad (\sigma \varphi)^{m} = \frac{\partial L}{\partial \varphi_{m,i}},
\]

which contain the physical momenta (i.e., along \( n_i = \delta^0_i \))

\[
\pi = \pi^{(0)} = \frac{\partial L}{\partial \dot{\varphi}} - (\partial L / \partial \dot{\varphi} \sigma \varphi), \quad p^m = p^{m(0)} = \frac{\partial L}{\partial \dot{\varphi} \varphi_m},
\]

where the dot denotes partial time derivation. Note that we use latin letters for spacetime indices and greek letters for spatial indices (and zero for the time component). Further, we take the convention that expressions of the form \( \partial L / \partial \dot{\varphi}_{i,0} \), or equivalently, \( \partial L / \partial \varphi_{i,m} \), are always to be interpreted as the component \( m = 0 \) of the initial expression \( \partial L / \partial \varphi_{i,m} \). (This is very important, for instance if \( L = \varphi_{i,m} \varphi^{m,m} \). With our convention, we have \( \partial L / \partial \varphi_{m,0} = 2 \varphi^{m,0} \), although the mixed term \( \varphi_{m,0} \varphi^{m,0} \) is actually contained twice in \( L \).)

The stress-energy tensor \( \pi_m^{(k)} \) can now be written in the form

\[
\tau^k_i = \pi^{(k)} \varphi_i + p^{m(k)} \psi_{m,i} - \delta^k_i L,
\]

where it is tempting to see in \( \psi_m \equiv \varphi_{m,i} \) the variable canonically conjugate to \( p^{m(i)} \). Further, the identically conserved form of the stress-energy tensor from [3] takes the form

\[
\tau^k_i = \frac{1}{2} \left[ \pi^{(m)} (\sigma \varphi)^k \right]_{i,m},
\]

where \( (\sigma \varphi)^k_i = 2 \delta^k_i \varphi_i + [(\sigma \varphi)^k]_{i,j} \), i.e., it acts correctly on \( \psi_j \) in accordance with its total tensor structure, taking account of the additional vector index.

The last relation holds only in generally covariant theories (e.g., General Relativity), and is given here only to demonstrate how naturally one is led to the specific choice of canonical variables. For the moment, we confine ourselves to special relativistic theories.

The conserved momentum is given as integral over a three dimensional hypersurface, \( \mathcal{P}_i = \int \tau^k_i d\sigma_k \). For \( n_i = \delta^0_i \), this is simply \( \mathcal{P}_i = \int \pi^{(0)} d^3 x \). We see that only the physical momenta \( m \) enter that expression. In particular, for the field energy \( \mathcal{H} = \mathcal{P}_0 \), we find

\[
\mathcal{H} = \int \left[ \pi \dot{\varphi} + p^m \psi_m - L \right] d^3 x,
\]
where we use already the letter $H$ although we yet have to eliminate the velocities.

Until this point, we have done nothing but written down the canonical field energy in terms of certain variables. Whether or not we can indeed interpret $\varphi, \pi$ and $\psi_m, \pi^m$ as canonical phase space variables and whether or not $H$ generates the time evolution of those variables is still an open question. However, from the above relations, any different choice of variables would seem unnatural.

The conventional Hamiltonian formulation of second order theories is based on two pairs of canonically conjugated variables, $\varphi, \pi$ and $\psi, \pi$, with $\psi = \dot{\varphi}$. This method goes back to Ostrogradski. We will investigate the relation between both methods at a later stage of this paper. Let us just remark that the fact that we use more variables should ultimately result in a theory with more constraints. If this is not the case, then both methods cannot be equivalent.

Finally, we assume the following equal-time Poisson brackets

$$[\varphi(x), \pi(y)] = \delta(x - y), \quad [\psi_m(x), p^k(y)] = \delta^k_m \delta(x - y), \quad (9)$$

and zero for any other bracket, e.g., $[\varphi, \psi_m] = 0$. For simplicity, we use $x, y$ to denote the space points $x^\mu, y^\mu$, and $\delta(x - y) = \delta^{(3)}(x - y)$ for the three dimensional delta function. The covariant form (i.e., with respect to a general, unspecified hypersurface) of those relations are given in [2]. Note that even classically, the relations (9) cannot be verified. It is indeed possible to construct the Poisson bracket such that it gives canonical relations for an arbitrary choice of variables. The only thing subject to verification is the resulting Hamiltonian theory. To this we turn now.

In the next two sections, we will apply the above formalism to several simple second order scalar field Lagrangians. It turns out that in all cases, the formalism reveals itself to be consistent. In section 4, we briefly analyze the relation to the conventional Ostrogradski formalism. Finally, in section 5, we treat General Relativity as a constrained second order theory and in section 6, we briefly discuss the relation of the first class constraints to the diffeomorphism invariance of the theory.

## 2 Unconstrained theories

As a first example, we consider the Lagrangian

$$\mathcal{L} = \frac{1}{2} \varphi, i \varphi^i + \frac{1}{2} \Box \varphi \Box \varphi, \quad (10)$$

where we use the notation $\Box \varphi = \varphi^{,i} i$ and $\Delta \varphi = \varphi^{,\mu} \,_{\mu}$ ($\mu = 1, 2, 3$). The field equations are $\Box \Box \varphi - \Box \varphi = 0$. We do not discuss the physical relevance of such a theory (therefore, coupling constants have been omitted). The inclusion of a potential, in particular a mass term, is trivial and does not lead to significant modifications of our discussion. In what follows, we will refer to the theory based on the above Lagrangian as example I.

The momenta are found from (5) in the form

$$\pi = \dot{\varphi} - \Box \varphi, \quad p^m = \delta^m_0 \Box \varphi \quad (11)$$

It turns out to be convenient to simplify the notations for the time components of $p^m$ and $\psi_m = \varphi, m$, and to use $p^0 = p$ and $\psi_0 = \psi$. Thus, we have $\psi = \dot{\varphi}$ (as in the Ostrogradski formulation), as well as $\psi_\mu = \varphi, \mu$. Those three relations do not contain velocities, and must therefore be considered as constraints. Next, we have $p = \Box \varphi = \dot{\psi} + \Delta \varphi$ and $\pi = \psi - \dot{p}$, both containing velocities, as well as $p^0 = 0$, which are constraints again.

As a result, we have the following 6 constraints

$$\Phi_\mu = \psi_\mu - \varphi, \mu, \quad \Psi^\mu = p^\mu, \quad (12)$$

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which satisfy
\[ [\Phi_\mu, \Psi^\nu] = \delta^\nu_\mu \delta,\] (13)
as well as \([\Phi_\mu, \Phi_\nu] = [\Psi^\mu, \Psi^\nu] = 0\), where we omit the arguments for simplicity of the notation. Thus, we are dealing with second class constraints, which have to be dealt with by the introduction of the Dirac bracket (see [4]). For the specific structure (13), it is not hard to show that the Dirac bracket can be written in the form
\[ [A, B]^* = [A, B] + [A, \Phi_\mu][\Psi^\mu, B] - [A, \Psi^\mu][\Phi_\mu, B].\] (14)

Note that apart from a summation over \(\mu\), there is also an integration over the argument of \(\Phi_\mu(z)\) and \(\Psi^\mu(z)\) involved, which is suppressed by our simplified notation.

We now easily find the following Dirac bracket relations
\[ [\varphi, A]^* = [\varphi, A], \quad [\psi, A]^* = [\psi, A], \quad [\psi_\mu, \pi]^* = \delta_\mu, \quad [p, \pi]^* = 0, \quad [p^\mu, \psi_\nu]^* = 0,\] (15)
where \(A\) is arbitrary. As it turns out, the relations are exactly those that could have been assumed right from the start if one would not have considered \(\psi_\mu\) and \(p^\mu\) as canonical variables. This is rather a coincidence, however, as we will see in the next example. (The notation \(\delta_\mu\) is to be interpreted as \(f_\delta_\mu = -f_{,\mu}^\delta\) for a function \(f\). The omission of the arguments is not without danger. Note, for instance, that from \([\psi_\mu(x), \pi(y)] = \delta_\mu(x - y)\), we find \([\pi(y), \psi_\mu(x)] = -\delta_\mu(x - y) = \delta_\mu(y - x)\), and thus, in short notation, \([\pi, \psi_\mu] = \delta_\mu\), contrary to what could have been expected from the initial relation \([\psi_\mu, \pi] = \delta_\mu\) and the antisymmetry of the Poisson bracket.)

In any case, we can now impose the constraints as strong relations between the variables, and thus eliminate \(\psi_\mu\) and \(p^\mu\) as independent field variables. Then, we use (8) in order to write down the Hamiltonian. The velocities (of the remaining variables \(\varphi\) and \(\psi\)) are easily expressed in terms of the momenta as \(\dot{\varphi} = \psi\) and \(\dot{\psi} = p - \Delta \varphi\). We find
\[ H = \int (\pi \dot{\psi} + \frac{1}{2} p^2 - p \Delta \varphi - \frac{1}{2} \psi^2 - \frac{1}{2} \varphi_{,\mu} \varphi^{,\mu}) d^3x.\] (16)

With the help of (15), we find
\[ [H, \varphi]^* = -\psi = -\dot{\varphi}, \] (17)
\[ [H, \pi]^* = -\Delta p + \Delta \varphi = -(\Box \varphi - \Box \dot{\varphi}) - (\ddot{\varphi} - \Delta \dot{\varphi}) = -\dot{\pi}, \] (18)
\[ [H, \psi]^* = -p + \Delta \varphi = -\dot{\psi}, \quad [H, p]^* = \pi - \psi = -\dot{p}.\] (19)

Thus, the Hamiltonian does indeed generate the time evolution of the fields. To conclude, despite the fact that additional pairs of variables \((\psi_\mu, \pi^\mu)\) revealed themselves as irrelevant, the formalism has nevertheless successfully passed its first test.

We now start form the Lagrangian
\[ L = \frac{1}{2} \varphi_{,i} \varphi^{,i} + \frac{1}{2} \varphi_{,i,m} \varphi^{,i,m}.\] (20)

This theory, which will be referred to as \textit{example II}, is equivalent to the previous one in the sense that it leads to the same field equations. It differs, however, by a four divergence and therefore, differences in the Hamiltonian theory will arise. We find \(\pi = \dot{\varphi} - \Delta \varphi, \quad p^m = \dot{\varphi}^{,m}\), and thus, writing again \(\psi = \psi_0\) and \(p = p^0\), we have \(\pi = \dot{\psi} - p_{,\mu}^\delta - \dot{\rho}\) and \(p = \dot{\psi}\), which are relations involving velocities. In addition, we have the constraints
\[ \Phi_\mu = \psi_\mu - \varphi_{,\mu}, \quad \Psi^\mu = p^\mu - \psi_{,\mu}.\] (21)
which satisfy again \([\Phi_\mu, \Phi_\nu] = [\Psi_\mu, \Psi_\nu]\) and
\[
[\Phi_\mu, \Psi_\nu] = \delta_\mu^\nu \delta.
\] (22)

Although the constraints satisfy the same Poisson structure as in example I, they are nevertheless fundamentally different because of the explicit occurrence of \(\psi\). Indeed, we now find the following Dirac brackets
\[
[\phi, A]^* = [\phi, A], \quad [\psi, A]^* = [\psi, A], \quad [\psi_\mu, \pi]^* = \delta_\mu^\nu, \quad [p, \pi]^* = -\Delta \delta, \quad [p^\mu, \psi_\nu]^* = 0
\] (23)

for arbitrary \(A\). They are identical to (15), except for the relation \([p, \pi]^* = -\Delta \delta\), which is of course again a symbolic notation for \(f(\Delta \delta) = (\Delta f) \delta\). Imposing the constraints as strong relations in \(\mathcal{H}\), we find
\[
\mathcal{H} = \int (\pi \psi + \frac{1}{2} p^2 - \frac{1}{2} \varphi_i \varphi^i + \frac{1}{2} \varphi_\mu \varphi^{\mu} - \frac{1}{2} \varphi_\mu \varphi_\nu \varphi^{\mu \nu}) d^3x,
\] (24)

where the velocities have been eliminated by \(\dot{\psi} = p\) and \(\dot{\psi}_\mu = \pi_\mu = \psi_\mu\), as well as \(\dot{\phi} = \psi\). We now easily derive
\[
[\mathcal{H}, \phi]^* = -\dot{\psi} = -\dot{\phi}
\] (25)
\[
[\mathcal{H}, \pi]^* = -\Delta p + \Delta \varphi - \Delta \Delta \varphi = -\Delta \dot{\phi} + \Delta \varphi + \Delta \Delta \varphi = (\Box \varphi - \Box \Box \varphi) - (\dot{\phi} - \Box \dot{\varphi}) = -\dot{\pi},
\] (26)
\[
[\mathcal{H}, \psi]^* = -p = \dot{\psi}, \quad [\mathcal{H}, p]^* = \Delta \dot{\psi} + \pi - \psi = \dot{\pi}.
\] (27)

Again, the formalism works perfectly well. As before, the additional variables \((\psi_\mu, p^\mu)\) could be eliminated after the introduction of the Dirac brackets. It is expected that this is a general feature of our formalism, if there is any hope for it to be equivalent to the Ostrogradski formulation based on only two pairs of variables. On the other hand, it should be noted that, in contrast to example I, in the present case, we could not have anticipated the relation \([p, \pi]^* = -\Delta \delta\). If we simply ignore the variables \(\pi_\mu\) and \(\psi_\mu\), then this relation cannot be derived, since we need the complete set of constraints (21) to get the correct Dirac brackets. Finally, in order to avoid confusion, we should mention that in the title of this section, we use the term unconstrained in the sense that in the conventional Ostrogradski formulation, those theories are indeed free of constraints. In our modified formalism, there will always be at least those constraints that eliminate the variables \(\psi_\mu\) and \(p^\mu\). In a constrained theory, there will be additional constraints.

### 3 Constrained theory

We now consider the Lagrangian
\[
\mathcal{L} = \frac{1}{2} \varphi_i \varphi^i + \alpha \varphi \Box \varphi.
\] (28)

This theory (example III) is equivalent to the conventional first order scalar field theory and we can thus expect that the application of the second order formalism leads to a constrained system. The momenta are found in the form \(\pi = \varphi (1 - \alpha) = \psi (1 - \alpha)\) and \(p^\mu = \delta_\mu^\nu \alpha \varphi\). Thus, apart from the constraints
\[
\Phi_\mu = \psi_\mu - \varphi_\mu, \quad \Psi^\mu = p^\mu,
\] (29)
we now have the additional constraints
\[
\Phi = p - \alpha \varphi, \quad \Psi = \pi - (1 - \alpha) \psi.
\] (30)
since none of those relations involves velocities. The constraints are all second class. Rather than deriving directly the Dirac brackets for the system of those eight constraints (at each point $x$), it is convenient to proceed in two steps. First, we construct the Dirac bracket that eliminates the constraints (29). (The construction of the Dirac brackets by eliminating the constraints in two steps will be given at the end of this section.)

The constraints are identical to those of example I, and the result, as we have seen, is simply that we can eliminate the variables $\psi_\mu$ and $p^\mu$ in terms of $\varphi_\mu$. The Dirac brackets for the remaining variables are identical to the initial Poisson bracket, see (15). We will therefore retain the notation $[A, B]$.

In a second step, we turn to the constraints (30), which satisfy

$$[\Phi, \Psi] = (1 - 2\alpha)\delta.$$  

(31)

The corresponding Dirac bracket is easily shown to be of the form

$$[A, B]^* = [A, B] + \frac{1}{1 - 2\alpha}[A, \Phi][\Psi, B] - \frac{1}{1 - 2\alpha}[A, \Psi][\Phi, B],$$  

(32)

where again an integration is suppressed by our notation. We find the following relations

$$[\pi, \varphi]^* = -\frac{1 - \alpha}{1 - 2\alpha} \delta, \quad [\varphi, p]^* = [\pi, \psi]^* = 0, \quad [\pi, p]^* = -\alpha \frac{1 - \alpha}{1 - 2\alpha} \delta, \quad [\varphi, \psi]^* = \frac{1}{1 - 2\alpha} \delta.$$

(33)

The Hamiltonian is found from (8) upon imposing the constraints as strong relations. The result is

$$H = \int \left(\frac{1}{2} - \alpha\right) \pi^2 \left(\frac{1}{2} - \alpha\right) \varphi_\mu \varphi_\mu - \alpha(\varphi_\mu \varphi_\mu)_{,\mu}\right)d^3x.$$  

(34)

If we rescale the momentum $\pi$ by introducing $\hat{\pi} = \frac{1 - 2\alpha}{1 - \alpha} \pi$, such that $[\hat{\pi}, \varphi]^* = -\delta$, we can alternatively write

$$H = \int \left(\frac{1}{2} - \frac{1}{1 - 2\alpha} \hat{\pi}^2 - \frac{1}{2} - \alpha\right) \varphi_\mu \varphi_\mu - \alpha(\varphi_\mu \varphi_\mu)_{,\mu}\right)d^3x.$$  

(35)

Apart from the last term, which is a surface term, the Hamiltonian corresponds to the conventional first order Hamiltonian derived from $\mathcal{L} = \left(\frac{1}{2} - \alpha\right) \varphi_\mu \varphi_\mu$, which is equal to (28) up to a four divergence.

For the rest, the relations

$$[H, \varphi]^* = -\varphi, \quad [H, \pi]^* = -\hat{\pi}$$

(36)

are easily verified. Thus, our formalism works even for such a strongly constrained system.

The Lagrangian (28) for the specific value $\alpha = 1$ can be viewed as a toy model that mimics in some sense the Lagrangian of General Relativity. Namely, the Lagrangian $\sqrt{-g} R$ consists of a part containing only first derivatives of the metric and a part that contains the metric and its second derivatives (linearly). The second part equals, up to a four divergence, the double of the opposite of the first part, similarly as in (28) for $\alpha = 1$. It is indeed the scope of our exercise to provide a Hamiltonian formalism that can be applied to General Relativity in its explicitly covariant form, in contrast to the conventional first order method, where a surface term has to be omitted, resulting in an effective Lagrangian that is not explicitly covariant.

At first sight, this may look like an unnecessary complication, since the number of variables is initially increased only to be reduced again at a later stage by imposing the constraints. Nevertheless, it is hoped that despite those computational complications, there will be an improvement of clarity in particular concerning the physical meaning of the constraints of the theory. Indeed, it is well known that the primary and secondary first class constraints arising in generally covariant theories are directly related to diffeomorphism invariance.
It turns out that those constraints can be directly inferred by a straightforward analysis of the corresponding Noether currents (that is, the stress-energy tensor). The explicit form of the constraints and their action as generators of coordinate transformations has been given in [2] for first order theories, and similar relations are easily derived for second order theories, following along the same lines. On the other hand, if we work with an effective, not explicitly covariant Lagrangian, the relation between constraints and generators of coordinate transformations is more obscure and explicit calculations have to be performed in order to determine the action of the constraints on the fields. For instance, simple relations, like the symmetry properties of (3), are not valid anymore. There will be, of course, alternative relations expressing the (hidden) coordinate invariance, but those will not emerge directly from Noether’s theorem and have to be obtained more or less by guesswork.

A second, related, issue concerns the occurrence of surface terms in the Hamiltonian. In view of the specific asymptotic behavior of the metric, e.g., \( g_{00} = 1 - m/r \) (for asymptotically flat spacetimes), surface integrals occurring in General Relativity do not always vanish, in contrast to conventional field theories. In fact, it is not hard to show from (3) that the only field that explicitly contributes to the integrated field momentum is the gravitational field. This raises problems when the effective, first order Lagrangian is used in General Relativity, since the omission of four divergences in the Lagrangian ultimately leads to a modification of \( \mathcal{H} \) by surface terms, see, e.g., [5]. Initially, in the context of canonical quantum gravity, certain surface terms in the Hamiltonian where simply ignored, since they are dynamically irrelevant [5]. Later [6], it was recognized that by the omission of those surface terms, we actually omit the complete field energy of the system (such that the resulting Hamiltonian vanishes weakly) and it was argued, based on comparison with the linearized theory, that those terms should not be omitted (except for closed spaces). This was confirmed in [7], where it was shown that without those terms, the Hamiltonian formulation of the theory is classically inconsistent, because the variations \( \delta \mathcal{H}/\delta \varphi \) and \( \delta \mathcal{H}/\delta \pi \) cannot be properly defined if those terms are missing, and thus, we cannot write down the Hamiltonian equations of motion. For a discussion of the treatment of surface terms in the variational principle of field theory, see also [8] and [9].

Obviously, in view of this situation, it seems promising to start directly from the full Lagrangian \( \sqrt{-g} \, R \), instead of omitting first a four-divergence, and then eventually reintroduce it again (in the form of a three-divergence) into the Hamiltonian in order to get a consistent theory. With the use of the second order Hamiltonian formulation, it should be possible to proceed strictly canonically, without ever being in the need to omit or add a surface term. The resulting Hamiltonian can be interpreted directly as field energy and should generate the time evolution of the system, provided we are able to deal consistently with all the constraints. In asymptotically flat spacetimes, it does not vanish weakly. We will outline this procedure in section 5.

Since it might not be obvious that the construction of the Dirac brackets in two steps (namely, first eliminating the constraints (29) and then the constraints (30)) leads indeed to the same result than the construction following directly the procedure of Dirac, we close this section by giving a justification of this procedure for an arbitrary theory.

Suppose we have second class constraints \( \Psi^i, \Phi^\alpha \), where it is irrelevant whether the labels \( i, \alpha \) run over a finite set (index) or an infinite set (like the argument \( x \)). Let the Poisson brackets be given by

\[
[\Psi^i, \Psi^k] = C^{ik}, \quad [\Phi^\alpha, \Phi^\beta] = D^{\alpha\beta},
\]

with invertible, antisymmetric \( C^{ik}, D^{\alpha\beta} \), the inverse being denoted by \( C_{ik} \) and \( D_{\alpha\beta} \) respectively. Nothing is assumed for \( [\Psi^i, \Phi^\alpha] \). They may or may not vanish.

Let \( A, B \) be any expression of the canonical variables (fields (or coordinates) and momenta). Then, in a first step, we define

\[
[A, B]^* = [A, B] - [A, \Psi^i]C_{ik}[\Psi^k, B],
\]

from which we easily find \( [A, \Psi^m]^* = [\Psi^m, B]^* = 0 \) for any of the \( \Psi^m \)'s and for arbitrary \( A, B \).
In a second step, define
\[ [A, B]^{**} = [A, B]^* - [A, \Phi^\alpha]^* D_{\alpha\beta}[\Phi^\beta, B]^*. \]

Obviously, we have \([A, \Phi^\gamma]^{**} = [\Phi^\gamma, B]^{**} = 0\) for any of the \(\Phi^\alpha\)'s and for arbitrary \(A, B\). But since we also have \([A, \Psi^i]^* = [\Psi^i, B]^* = 0\) for any \(A, B\) (and thus, in particular, e.g., \([\Psi^i, \Phi^\alpha]^* = 0\)), we find that trivially \([A, \Psi^i]^{**} = [\Psi^i, B]^{**} = 0\) for any \(A, B\).

Moreover, from the above construction, it is also clear that for those \(A, B\) that commute with all of the constraints (i.e., \([A, \Psi^i] = [A, \Phi^\alpha] = 0\), and similar for \(B\)), we have \([A, B]^{**} = [A, B]\).

Summarizing, the bracket \([\cdot, \cdot]\)^** has the following properties: (1) \([A, \Xi^M]^{**} = 0\) for all of the second class constraints \(\Xi^M = (\Psi^i, \Phi^\alpha)\) and for arbitrary \(A\). (2) If \(A, B\) commute with all of the constraints \(([A, \Xi^M] = [B, \Xi^M] = 0\)), then \([A, B]^{**} = [A, B]\). But those are exactly the properties that define the Dirac bracket.

In other words, the bracket \([\cdot, \cdot]\)^** has exactly the same properties as the bracket
\[ [A, B]^\# = [A, B] - [A, \Xi^M] E_{MK} [\Xi^K, B], \]

where \(E^{MK} = [\Xi^M, \Xi^K]\), and \(E_{MK}\) the inverse of \(E^{MK}\). But since the bracket defined by the above properties (1) and (2) is unique, we must have \([A, B]^\# = [A, B]^{**}\). There is thus no need to show this explicitly.

This justifies the two step construction of the Dirac brackets.

### 4 Original Ostrogradski formulation

We started our investigation from the explicit expression of the canonical stress-energy tensor. From its structure, it was most natural to introduce \(\varphi\) and \(\psi_m = \varphi_m\) as independent variables and to base the canonical Hamiltonian formalism on that. On the other hand, the canonical stress-energy tensor is not the only conserved current available. As is well known, arbitrary relocalization terms can be added to \(\tau^k_{i,k}\) without changing the relation \(\tau^k_{i,k} = 0\). In special relativistic theories, not even the integrated momentum is changed by such a procedure. (Gravity, however, provides an exception to this, because of the previously mentioned different asymptotic behavior.) In view of those ambiguities concerning in particular the energy density, it is not really surprising that there may also exist several Hamiltonians for one and the same theory.

There is a simple way to get at least to two of such Hamiltonian descriptions. As is well known, in first order theory, the momentum can be derived directly from variation of the action functional as \(\delta S/\delta \varphi = \partial L/\partial \dot{\varphi} = \pi\). Here, the notation \(\delta A\) denotes a three dimensional variation, i.e., if we find for the variation of a functional \(A(\varphi, \pi)\) that \(\delta A = \int (a_1 \delta \varphi + a_2 \delta \pi) d^3x\), then by definition, \(a_1 = \delta A/\delta \varphi\) and \(a_2 = \delta A/\delta \pi\). It turns out that in second order theories, a similar variation of the action does not lead to a unique definition of the canonical momenta. Indeed, we have
\[
\delta S = \int \left( \frac{\partial L}{\partial \dot{\varphi}} \delta \varphi + \frac{\partial L}{\partial \varphi_i} \delta \varphi_i + \frac{\partial L}{\partial \varphi_{i,k}} \delta \varphi_{i,k} \right) dt \, d^3x. \quad (37)
\]

Using the field equations \(\partial L/\partial \varphi = (\partial L/\partial \varphi_{i,i})_i - (\partial L/\partial \varphi_{i,i,k})_i,k\) in the first term, then performing several partial integrations, where three divergences can be omitted (surface terms), while the time integration over time derivatives can be carried out explicitly, one readily finds
\[
\delta S = \int \left( \left( \frac{\partial L}{\partial \dot{\varphi}} - \frac{\partial L}{\partial \varphi_{i,i}} \right)_i \delta \varphi + \frac{\partial L}{\partial \varphi_i} \delta \varphi_i \right) d^3x, \quad (38)
\]
which leads exactly to our previously adapted choice of fields and momenta
\[
\frac{\delta S}{\delta \varphi} = \frac{\partial L}{\partial \dot{\varphi}} - \left( \frac{\partial L}{\partial \dot{\varphi},i} \right)_i \equiv \pi, \quad (39)
\]
\[
\frac{\delta S}{\delta \varphi,i} = \frac{\partial L}{\partial \dot{\varphi},i} \equiv p^i. \quad (40)
\]

On the other hand, one can also do with less variables. Writing the integrand of the second contribution in (38) in the form \(\left( \frac{\partial L}{\partial \dot{\varphi},i} \right)_i \delta \varphi - \left( \frac{\partial L}{\partial \dot{\varphi},i} \right) \delta \varphi,i \equiv \pi\), then omitting in the first term of this expression the three divergence and carrying out the time differentiation, we find
\[
\delta S = \int \left( \left[ \frac{\partial L}{\partial \dot{\varphi},i} - \left( \frac{\partial L}{\partial \dot{\varphi},i} \right)_i \right] \delta \varphi + \frac{\partial L}{\partial \ddot{\varphi}} \delta \dot{\varphi} \right) d^3x, \quad (41)
\]
which leads to
\[
\frac{\delta S}{\delta \dot{\varphi}} = \frac{\partial L}{\partial \dot{\varphi}} - 2 \left( \frac{\partial L}{\partial \dot{\varphi},\mu} \right)_\mu \equiv \tilde{\pi}, \quad (42)
\]
\[
\frac{\delta S}{\delta \ddot{\varphi}} = \frac{\partial L}{\partial \ddot{\varphi}} \equiv \tilde{p}, \quad (43)
\]
that is, to a theory with variables \((\varphi, \psi = \dot{\varphi})\) and corresponding momenta \((\tilde{\pi}, \tilde{p})\). Writing down the Hamiltonian for this theory, that is,
\[
\tilde{H} = \int (\tilde{\pi} \ddot{\varphi} + \tilde{p} \dot{\psi} - \mathcal{L}) d^3x, \quad (44)
\]
and comparing it with our initial Hamiltonian \(H = \int (\pi \ddot{\varphi} + p^m \dot{\psi}_m - \mathcal{L}) d^3x\), we find that the difference is given by a surface term
\[
H = \tilde{H} + \int \left( \frac{\partial L}{\partial \dot{\varphi},\mu} \right)_\mu d^3x = \tilde{H} + \oint \frac{\partial L}{\partial \dot{\varphi},\mu} \dot{\varphi} d\sigma_\mu. \quad (45)
\]
In as far surface terms are assumed to vanish (as has been assumed during the derivation of (38) and (41)), both expressions are equal. This does still not mean that the corresponding Hamiltonian theories are also equivalent.

The formulation based on treating the velocities as independent fields is known as Ostrogradski formulation, see, e.g., [10] and [11] and in particular [12], where the formalism has been adapted from the case of a finite number of variables to the case of field theory. (The point is that in the finite case, their is no such thing as a spatial derivative, and the distinction between the above presented formulations cannot be done anyway.)

Let us briefly verify the consistency of the formulation based on \(\tilde{H}\) for the three examples we previously dealt with in the alternative formulation. It seems obvious that for the cases of the Lagrangian [10] (example I), as well as for the constrained theory [28] (example III), both formulations are trivially equivalent, because of the absence of mixed derivatives \(\varphi_{,\mu,0}\). Indeed, we have for those cases \(p = \tilde{p}\) and \(\pi = \tilde{\pi}\), while the variables \(\psi_{,\mu}\) and \(p^\mu\) could be eliminated without any changes of the Poisson brackets between the remaining variables.

Only the case [20] (example II) deserves closer examination. We find from [12] and [43] the momenta \(\tilde{p} = \dot{\varphi} = \dot{\psi}\) and \(\tilde{\pi} = \psi - 2\Delta \dot{\varphi} - (\dot{\varphi}) = \psi - 2\Delta \psi - \dot{\tilde{p}}\). The system is thus free of constraints. The Hamiltonian [14] takes the form
\[
\tilde{H} = \int (\tilde{\pi} \psi + 1/2 \ddot{p}^2 - 1/2 \psi^2 - 1/2 \varphi_{,\mu} \varphi^{,\mu} - \dot{\psi}_{,\mu} \psi^{,\mu} - 1/2 \varphi_{,\mu,\nu} \varphi^{,\mu,\nu}) d^3x, \quad (46)
\]
where the velocities have been eliminated with $\dot{\phi} = \psi$ and $\dot{\psi} = \tilde{p}$. It is needless to say that the only non-vanishing fundamental Poisson brackets in the present formalism are assumed to be

$$[\tilde{\pi}, \phi] = -\delta, \quad [\tilde{p}, \psi] = -\delta.$$  \hspace{1cm} (47)

Note, by the way, that if we compare with the momenta of the alternative formulation of section 2, we have $\tilde{p} = p$ and $\tilde{\pi} = \pi - \Delta \psi$. Therefore, from the above Poisson bracket, we can directly derive the relation $[p, \pi] = -\Delta \delta$ that arose in the other formulation upon defining the Dirac brackets (see (23)).

Next, from (46), we find

$$[\tilde{H}, \phi] = -\psi = -\dot{\phi}, \quad [\tilde{H}, \psi] = -\tilde{p} = -\dot{\psi},$$  \hspace{1cm} (48)

as well as

$$[\tilde{H}, \tilde{\pi}] = \Delta \varphi - \Delta \Delta \varphi = -\tilde{\pi}, \quad [\tilde{H}, \tilde{p}] = -\dot{\tilde{\pi}} = -\dot{\tilde{p}},$$  \hspace{1cm} (49)

where the field equations have been used in the first relation. Thus, the Hamiltonian $\tilde{H}$ generates indeed the time evolution of the phase space variables $\phi, \psi, \tilde{\pi}$ and $\tilde{p}$.

To conclude, we see that both the initial Ostrogradski formulation, as well as our modified formulation, lead to consistent Hamiltonian theories for the simple models analyzed here. Numerically, the corresponding Hamiltonians differ by a surface integral.

As outlined at the end of the previous section, we expect certain improvements of clarity by the use of our modified formulation. Although the Hamiltonian formulation necessarily induces a 3+1 split of spacetime, it seems nevertheless in the spirit of a covariant theory to treat $\varphi, \mu$ and $\dot{\phi}$ in a symmetric way, at least initially. One advantage of such a procedure has already been encountered: The resulting Hamiltonian is directly given by the integrated time component of the canonical stress-energy tensor, i.e., by the time component of the four-momentum $P_i = \int \tau^t \delta \sigma_k$. On the other hand, the Ostrogradski Hamiltonian is not a component of anything (it corresponds rather to a generalized Legendre transform of the Lagrangian), and its conservation as well as its identification with the energy have to be established separately. A direct relation to the stress-energy tensor, and thus to the Noether current corresponding to the translational invariance of the theory, should turn out to be profitable in generally covariant theories, where we will have to deal with constraints related to diffeomorphism invariance (see [2]).

5 General Relativity

We start from the Lagrangian

$$\mathcal{L} = \sqrt{-g}R,$$  \hspace{1cm} (50)

where for simplicity, we omit the factor $-\frac{1}{2}$ which is necessary to get the correct sign for the energy. The field variables, in the second order formalism, are $g_{ik}$ and $\psi_{ikm} = g_{ik,m}$. Further, we find from (5)

$$\pi^{ik} = \frac{\sqrt{-g}}{2} \left[ -\Gamma^i_{lm} g^{lm} g^{k0} - \Gamma^k_{lm} g^{lm} g^{i0} + \Gamma^i_{lm} g^{l0} g^{km} + \Gamma^k_{lm} g^{l0} g^{im} \right],$$  \hspace{1cm} (51)

$$p^{ikm} = \frac{\sqrt{-g}}{2} \left[ g^{i0} g^{km} + g^{k0} g^{im} - 2 g^{ik} g^{0m} \right].$$  \hspace{1cm} (52)

The Poisson brackets are assumed to be

$$[g_{ik}, \pi^{lm}] = \delta^{lk}_{lm} \delta_i^m, \quad [\psi_{ikq}, \pi^{lmr}] = \delta^{lk}_{lm} \delta^i_q \delta_{ir},$$  \hspace{1cm} (53)
where we use the familiar notation \( \delta_{ik}^{lm} = \frac{1}{2} (\delta^i_l \delta^m_k + \delta^i_k \delta^m_l) \).

We use again the simplified notation \( p^{ik} = p^{ik0} \) and \( \psi_{ik} = \psi_{ik0} = g_{ik0} \). Obviously, the relations (55) and (56) are all constraints, since the momenta are expressed in terms of \( \psi_{ikm} \) and \( g_{ik} \) (and not in terms of velocities). In addition, we have the constraints \( \psi_{ik \mu} = g_{ik \mu} \) (recall that greek indices run from 1 to 3). As a result, we have a total of 80 constraints, and at first sight, most of them seem to be second class. Surprisingly enough, with a little bit of patience, the above system can be handled without major difficulties.

Similar as in example III, we divide the constraints into two groups, with the first group consisting of

\[
\Phi_{ik \mu} = \psi_{ik \mu} - g_{ik \mu}, \quad (54)
\]

while the second group contains the remaining constraints,

\[
\Phi^{ik} = \pi^{ik} - \sqrt{-g} \left[ -\Gamma^i_{lm} k^m + \Gamma^k_{lm} k^0 + \Gamma^m_{lm} g^{ik0} - \Gamma^k_{lm} g^{im} \right], \quad (56)
\]

\[
\Psi^{ik} = p^{ik} - \sqrt{-g} \left[ g^{ik0} - g^{ik0} \right]. \quad (57)
\]

We begin with the first group. Those constraints satisfy

\[
[\Phi_{ik \mu}, \Psi^{lm \nu}] = \delta_{lm}^{ik} \delta_{\mu}^{\nu}, \quad (58)
\]

as well as \([\Phi_{ik \mu}, \Phi^{lm \nu}] = [\Psi^{ik \mu}, \Psi^{lm \nu}] = 0\). This is very similar to our previous examples, and the corresponding Dirac bracket reads

\[
[A, B]^* = [A, B] + [A, \Phi_{ikm}] [\Psi^{ikm}, B] - [A, \Psi^{ikm}] [\Phi_{ikm}, B], \quad (59)
\]

as is easily verified. (One has to check that the Dirac brackets between any quantity and any of the (above) constraints vanishes.) We can now eliminate the variables \( \psi_{ik \mu} \) and \( p^{ik \mu} \) by imposing the constraints as strong relations. It is not hard to verify from (59) that for the remaining variables, we have again that the Dirac bracket is identical to the initial Poisson bracket. Indeed, we have \([A, g_{ik}]^* = [A, g_{ik}], [A, \psi_{ik}]^* = [A, \psi_{ik}]\) for any \(A\) etc., see the corresponding relations (15) of section 2. In particular, we can also check that \([\pi^{ik}, p^{lm}]^* = 0\), just like in examples I and III.

To conclude, the 60 constraints (54) and (55) can be imposed strongly (that is, \(\psi_{ik \mu} \) and \(p^{ik \mu}\) are eliminated), and the remaining brackets remain unchanged. As in example III, we will denote them again by \([A, B]\), without star.

We are thus left with the 20 constraints (56) and (57). At this stage, the phase space variables are \(g_{ik}, \psi_{ik}, \pi^{ik}\) and \(p^{ik}\). Most constraints turn out to be second class (note that some components of \(\Gamma^i_{kl}\) depend on \(\psi_{ik} = g_{ik0}\) and have non-vanishing brackets with \(p^{ik}\)). The explicit calculations are quite long, and we will only present partial results here. First, we notice that we have

\[
[\Psi^{ik}, \Psi^{lm}] = 0. \quad (60)
\]

Further, we can derive the relations,

\[
[\Phi^{ik}, \Psi^{lm}] = [\Psi^{ik}, \Phi^{lm}] = 0. \quad (61)
\]

In particular therefore, \(\Phi^{ik}\) is first class. Let us write the remaining brackets in the form

\[
[\Phi^{\lambda \delta}, \Psi^{\mu \nu}] = G^{\lambda \delta \mu \nu} \delta_{\nu}, \quad [\Phi^{\lambda \delta}, \Phi^{\mu \nu}] = H^{\lambda \delta \mu \nu} \delta. \quad (62)
\]
There are further non-vanishing brackets $[\Phi^\mu,\Phi^\nu]$ and $[\Phi^{0i},\Phi^{0j}]$, for which we do not introduce specific symbols. Note, however, that $\Phi^{0i}$ are not first class. It is relatively easy to show that $G^{\lambda\delta\mu\nu}$ is given by the following expression

$$G^{\lambda\delta\mu\nu} = \sqrt{-g} \left[ \frac{1}{2} g^{\lambda\mu} g^{\delta\nu} - \frac{1}{2} g^{\lambda\nu} g^{\delta\mu} + \frac{1}{2} g^{\lambda\mu} g^{\delta\nu} g^{00} + \frac{1}{2} g^{\delta\mu} g^{00} - g^{\lambda\mu} g^{\delta\nu} g^{00} \right], \quad (63)$$

where the right hand side has still to be symmetrized with respect to $\mu\nu$ as well as with respect to $\delta\lambda$. At this point, it is convenient to introduce the Arnowitt-Deser-Misner parameterization of the metric, that is, we write $g_{00} = N^2 - \tilde{g}_{\mu\nu} N^\mu N^\nu$, $g_{0\mu} = -N_\mu$ and $g_{\mu\nu} = -\tilde{g}_{\mu\nu}$, where $N^\mu = \tilde{g}^{\mu\nu} N_\mu$, with $\tilde{g}^{\mu\nu}$ defined as inverse of $\tilde{g}_{\mu\nu}$. We can now write

$$G^{\lambda\delta\mu\nu} = -\frac{1}{2} N^{-1} \sqrt{g} \left[ \tilde{g}^{\lambda\delta} \tilde{g}^{\mu\nu} - \frac{1}{2} \tilde{g}^{\lambda\nu} \tilde{g}^{\delta\mu} - \frac{1}{2} \tilde{g}^{\lambda\mu} \tilde{g}^{\delta\nu} \right]. \quad (64)$$

Quite interestingly, this is (up to a factor $N^{-1}$) the same metric that appears in the Laplace-Beltrami type term of the Wheeler-DeWitt equation (the so-called superspace metric), see [6]. Let us also define the inverse metric

$$G_{\lambda\delta\mu\nu} = \frac{N}{\sqrt{g}} \left[ \delta_{\delta\mu} \tilde{g}_{\lambda\nu} + \tilde{g}_{\delta\nu} \tilde{g}_{\lambda\mu} - \tilde{g}_{\delta\lambda} \tilde{g}_{\mu\nu} \right], \quad (65)$$

satisfying

$$G_{\lambda\delta\mu\nu} G^{\mu\nu\alpha\beta} = \delta^{\alpha\beta}. \quad (66)$$

As to the other brackets in (62), we will not derive them explicitly here. In fact, $H^{\mu\nu\lambda\delta}$ does not simplify a lot. Note that $H^{\mu\nu\lambda\delta}$ is antisymmetric with respect to the exchange of the pairs of indices $\mu\nu$ and $\lambda\delta$ (in contrast to $G^{\mu\nu\lambda\delta}$, which is symmetric).

Having already identified $G_{\mu\nu\lambda\delta}$ as metric, we define $H_{\mu\nu\lambda\delta}$ as

$$H_{\mu\nu\lambda\delta} = G_{\mu\nu\alpha\beta} H^{\alpha\beta\rho\sigma} G_{\gamma\rho\lambda\delta}. \quad (67)$$

We introduce the following Dirac bracket

$$[A, B]^* = [A, B] + [A, \Phi^\mu] G_{\mu\nu\lambda\delta} [\Psi^{\lambda\delta}, B] - [A, \Psi^{\mu\nu}] G_{\mu\nu\lambda\delta} \left[ \Phi^{\lambda\delta}, B \right] - [A, \Psi^{\mu\nu}] H_{\mu\nu\lambda\delta} [\Psi^{\lambda\delta}, B]. \quad (68)$$

As always, integration over the arguments of the constraints is understood. It is not hard to verify that we have $[\Phi^\mu, A]^* = [\Psi^{\mu\nu}, A]^* = 0$ for any $A$. In particular we now have $[\Psi^{\mu\nu}, \Phi^{0i}]^* = 0$. We can also verify the relation $[\Phi^{0i}, \Phi^{0j}]^* = 0$. As a result, $\Phi^{0i}$ are now first class constraints. (This means that the group of constraints (60) and (61), in fact contained 4 first class constraints, but we did not recognize them prior to the introduction of the Dirac brackets, because we did not consider the correct combination of the constraints.)

All the second class constraints have now been eliminated, and the remaining set of variables can be chosen to be $(g_{\mu\nu}, \psi_{\mu\nu}, \psi_{0i}, \pi^{0i}, \psi_{0i}, p^{0i})$. Note that we have chosen $\psi_{\mu\nu}$ instead of $\pi^{\mu\nu}$, because it is easier to eliminate $\pi^{\mu\nu}$ than $\psi_{\mu\nu}$ (see [59]). This is, however, merely a matter of convenience, and once we have explicitly evaluated the Dirac brackets (68) between all the variables, we can easily reintroduce $\pi^{\mu\nu}$ at any stage. We will not perform this task completely here, but a few relations will be given below.

The canonical Hamiltonian is constructed from

$$\mathcal{H} = \int \left( \pi^{ik} \dot{\psi}_{ik} + p^{ikm} \dot{\psi}_{ikm} - L \right) \, d^3x, \quad (69)$$
which has to be expressed in terms of \((g_{\mu\nu}, \psi_{\mu\nu}, g_{0i}, \pi_{0i}, \psi_{0i})\). Taking into account the first class constraints \(\Phi^{0i}\) and \(\Psi^{0i}\), we find for the total Hamiltonian

\[
H_T = \mathcal{H} + \int \left( \lambda_i \Phi^{0i} + \mu_i \Psi^{0i} \right) d^3x.
\]

From this Hamiltonian, properly expressed in terms of the independent variables, together with the Dirac brackets (68), we can check for eventual secondary constraints. Note that \(\Psi^{0i} = \rho^{0i}\). It turns out that \(\rho^{0i}\) commutes with the Hamiltonian and does not generate secondary constraints. On the other hand, \(\Phi^{0i}\) will generate four secondary constraints, the so-called Hamiltonian constraints. The explicit calculations are straightforward, but rather lengthy, and will not be carried out here.

Nevertheless, we will give one Dirac bracket explicitly, in order to compare with the corresponding result of the conventional first order approach. As is easily shown, we have \([\Phi^{\mu\nu}, \psi_{\lambda\delta}] = 0\) as well as \([\Psi^{\mu\nu}, g_{\lambda\delta}] = 0\). Further, we find \([\Psi^{\mu\nu}, \psi_{\lambda\delta}] = -\delta_{\lambda\delta}^\mu\nu\) and \([\Phi^{\mu\nu}, g_{\lambda\delta}] = -\delta_{\lambda\delta}^{\mu\nu}\). From those relations, we can evaluate the Dirac bracket

\[
[\psi_{\alpha\beta}, g_{\mu\nu}]^* = G_{\alpha\beta\mu\nu}^\delta.
\]

We recall that the Dirac bracket is the starting point for the transition to the second quantized theory (see [4]). Therefore this relation (which becomes ultimately the commutator between \(\dot{g}_{\mu\nu}\) and \(g_{\mu\nu}\)) has to be valid independently of the specific choice of variables. Thus, the same relation should hold in the conventional first order approach, if only \(\dot{g}_{\mu\nu}\) is expressed in terms of the corresponding phase space variables.

Indeed, in the first order approach, we have [6]

\[
\pi^{\mu\nu}_1 = -\sqrt{\tilde{g}} (K^{\mu\nu} - \tilde{g}^{\mu\nu} K),
\]

where the subscript \((1)\) refers to the choice of variables in the first order approach. \(K_{\mu\nu}\) is defined as

\[
K_{\mu\nu} = \frac{1}{2} N^{-1}(N_{\mu,\nu} + N_{\nu,\mu} - \dot{\tilde{g}}_{\mu\nu}).
\]

This can be inverted to

\[
\dot{\tilde{g}}_{\mu\nu} = 2 \frac{N}{\sqrt{\tilde{g}}} \left( \pi^{\alpha\beta}_{(1)} - \frac{1}{2} \pi^{\gamma\delta}_{(1)} \tilde{g}_{\gamma\delta} \tilde{g}^{\alpha\beta} \right) \tilde{g}_{\alpha\mu} \tilde{g}_{\beta\nu} + \ldots
\]

where the dots indicate that there are additional terms, that do not depend on the momenta \(\pi^{\alpha\beta}_{(1)}\). The Poisson brackets in the first order theory are assumed to be \([\pi^{\alpha\beta}_{(1)}, \tilde{g}_{\mu\nu}]_{(1)} = -\delta_{\mu\nu}^{\alpha\beta}\). It is now an easy task to derive the symbolic relation

\[
[\tilde{g}_{\alpha\beta}, g_{\mu\nu}]_{(1)} = G_{\alpha\beta\mu\nu}^\delta,
\]

which holds if \(\dot{g}_{\alpha\beta}\) is expressed properly in terms of \(\pi^{\alpha\beta}_{(1)}\). (Note that \(g_{\mu\nu} = \tilde{g}_{\mu\nu}\) in the signature convention of [6], and \(g_{\mu\nu} = -\dot{\tilde{g}}_{\mu\nu}\) in our convention, but this difference is obviously not relevant for the final relation.) We conclude that both approaches ultimately lead to the same commutator between \(g_{\mu\nu}\) and \(\dot{g}_{\mu\nu}\). This provides strong evidence that the elimination of the second class constraints has been done consistently.

6 Discussion

In the previous section, we have treated General Relativity as a constrained second order field theory. We could successfully eliminate the second class constraints and the resulting theory is quite similar to the conventional
first order approach, containing 8 primary first class constraints, 4 of which are trivial and are expected not to lead to secondary constraints, while the remaining 4 are expected to lead to the so-called Hamiltonian constraints, similar as in the conventional approach.

What we have gained at this point is simply the fact that the Hamiltonian equals by construction the canonical field energy, including all eventual surface terms. It is important that, in order to achieve this, it is not only necessary to use a second order formalism, but rather to use our specific, modified formalism, since, as we have outlined in section 4, the conventional Ostrogradski Hamiltonian differs by a surface term from the canonical energy.

The fact, however, that the second order formulation allows us to start from the manifestly covariant Lagrangian $\sqrt{-g} R$ leads to further simplifications. As outlined in [2], the primary as well as the secondary first class constraints related to diffeomorphism invariance can be found by inspection of the Noether currents. Indeed, as a consequence of Noether’s theorem, for a generally covariant second order theory, four relations can be derived merely from invariance under coordinate transformations $x^i \rightarrow x^i + \xi^i$, see [1]. They are obtained by a successive localization of the coordinate translations [2]. The first, obtained from $\xi^i = \varepsilon^i = \text{const}$, is the conservation of $\tau^k_{\ i}$ in the form (2), i.e., $\tau^k_{\ i,k} = 0$. The second, obtained from $\xi^i = \varepsilon^i_k x^k$ with constant $\varepsilon^i_k$, allows for $\tau^k_{\ i}$ to be written in the form (3). The third and fourth, from $\xi^i = \varepsilon^i_{km} x^k x^l x^m$ respectively, lead to the mentioned symmetry properties of the brackets in the expression (3).

Those relations, when integrated over a spacelike hypersurface, lead directly to the first class constraints that arise as a result of the same symmetries. Let us start with the last one, i.e.,

$$\int \left( \frac{1}{2} \left[ \frac{\partial L}{\partial \dot{\varphi}^0} (\sigma_{\varphi})^0_{,i} \right] \right) d\sigma_k.$$  

As a result of diffeomorphism invariance, the totally symmetric part in $mlk$ of the integrand vanishes (see [2] for details). If we choose again $n_k = \delta^0_k$ for the normal vector to the hypersurface, then we must have

$$\int \left( \frac{1}{2} \left[ \frac{\partial L}{\partial \dot{\varphi}^0} (\sigma_{\varphi})^0_{,i} \right] \right) d^3 x = 0,$$

or simply (omitting the factor 1/2 and the integration for simplicity)

$$p^0(\sigma_{\varphi})^0_{,i} = 0.$$  

(Recall that $p^{0(0)} = p^0$ in our notation, see (4) and (5).) In particular, for a symmetric tensor field, we have $(\sigma_{g_{lm}})^k_i = 2(\delta^k_{m} g_{li} + \delta^k_{l} g_{im})$, and we find

$$p^{lm0}(\sigma_{g_{lm}})^0_i = 4p^{m0} g_{im} = 0,$$

where we recall our additional convention $p^{0} = p$ and thus, for the tensor case, $p^{ik0} = p^{ik}$. As expected, this is equivalent to the primary first class constraint $\Psi^{0i} = p^{0i} = 0$, see (57).

Similarly, from the antisymmetry in $kl$ of the first bracket in (3), we find, integrating over $d\sigma_k$ and choosing $n_k = \delta^0_k$,

$$\int \left[ -\frac{\partial L}{\partial \dot{\varphi}_{0,0}} - \frac{1}{2} \frac{\partial L}{\partial \dot{\varphi}_{0}} (\sigma_{\varphi})^0_{,i} - \frac{\partial L}{\partial \dot{\varphi}_{m,0}} (\sigma_{\varphi})^0_{,i,m} \right] d^3 x = 0$$

Written in terms of momenta, we find

$$p_{\varphi, i} - \frac{1}{2}(\pi + p^{k}_{,k})(\sigma_{\varphi})^0_{,i} + p_m[(\sigma_{\varphi})^0_{,i,m} = 0$$

(80)
For the metric theory, this can be written in the form

\[ \pi^{0i} = -p^{0i},k - \frac{1}{2} p^{lm} g_{lm,k} g^{ki} - 2 p^{0km} g_{kl,m} g^{il}. \]  

(81)

If we eliminate \( p^{ikm} \) in terms of the dynamical variables (i.e., if we impose the second class constraints \( \Phi^{\mu\nu} \) and \( \Psi^{\mu\nu} \) from (54) and (55), as well as \( \Phi^{0i} = 0 \) from (56)), we find that the above relations are identical to the first class constraints \( \Phi^{0i} = 0 \) from (56). Note, however, that the constraints in the form (78) and (81) will arise in any covariant second order tensor theory, irrespective of the specific Lagrangian and of the eventual presence of additional (second class) constraints.

Thus, we have recovered the primary first class constraints directly from the Noether relations obtained in [2] from the successive localization of the coordinate translations \( x^i \rightarrow x^i + \xi^i(x) \).

Finally, the secondary first class constraints can be obtained from the fact that \( \tau^k_i \) can be expressed both in the canonical form (2) and in the form (3). In other words, for the canonical field momentum, we can write

\[ P_i = \int \tau^0_i d^3x \]

\[ = \int \left( \left[ \frac{\partial L}{\partial \varphi_{0,\alpha i}} \varphi_{0,\alpha i} - \frac{1}{2} \frac{\partial L}{\partial \varphi_{m,0}} (\sigma \varphi)^0_{0,m} \right] + \frac{1}{2} \left[ \frac{\partial L}{\partial \varphi_{m,i}} (\sigma \varphi)^0_{0,m} \right] \right) d^3x. \]  

(82)

The expression in the second line is a surface term, as can be shown with the help of the symmetry properties of the brackets under the integral (see [2]). In order to express it in terms of the canonical momenta \( \pi \) and \( p^i \) (that is, to eliminate the terms containing \( \pi^{(\mu)} \) and \( p^{(\mu)} \) appearing in (82)), it is actually preferable to use first the symmetry properties and then integrate (that is, change first the order of the indices \( kl \) in the first term of (82) and then integrate, and similar for the second term). This is also necessary to find the generators of the coordinate transformations, see [2]. Again, the relation (82) is valid in any generally covariant second order theory.

In any case, we see that the secondary constraints express the fact that the canonical field momentum \( P_i \), and thus in particular the Hamiltonian \( H = P_0 \), is equal to a surface term. Just as in the conventional first order approach, the Hamiltonian vanishes weakly up to a surface term. While in the first order approach, this has to be checked explicitly, in our approach, it can be anticipated right from the start, since we work with an explicitly covariant Lagrangian, and can therefore make use of the full power of Noether’s theorem.

As a result, there is no need to explicitly evaluate the Hamiltonian in the form (69), because it will turn out to be weakly equal to the above surface term. All we have to do is to properly express (82) in terms of the dynamical variables, and to construct the Hamiltonian which will thus consist of a surface term and of the primary and secondary first class constraints derived previously.

The action of the constraints on the variables and their relation to the generators of spacetime translations are easily established following along the same lines as in [2], where the corresponding analysis has been carried out for first order theories. In contrast to our previous manipulations, i.e., the elimination of the second class constraints and the introduction of the Dirac brackets, which rely heavily on the Hilbert-Einstein Lagrangian, the discussion concerning the first class constraints and the generators of translations can be carried out in a general form and the results hold for any generally covariant second order field theory.

7 Conclusions

We have presented an alternative Hamiltonian formulation for field theories based on Lagrangians that contain second derivatives. This formulation differs from the conventional Ostrogradski formalism in that all four partial
derivatives of the field are considered as independent phase space variables, while in the Ostrogradski method, only the time derivative is considered in that way. In our formulation, the Hamiltonian is by construction equal to the canonical field energy, and will differ, in most cases, from the Ostrogradski Hamiltonian by a surface term. It turns out that the additional variables lead to second class constraints and can easily be eliminated with the help of the Dirac bracket. The formalism was applied successfully to several constrained and unconstrained second order scalar field theories and its equivalence (up to surface terms) to the Ostrogradski formulation was established. Finally, the full power of our formulation has been demonstrated by applying it to General Relativity. While conventionally, General Relativity is treated as first order theory, which leads to difficulties concerning certain surface terms that are omitted in the Lagrangian, but have to be reinserted into the Hamiltonian for consistency, the second order formalism allows us to work directly with the explicitly covariant Lagrangian. This way, we avoid not only the above problems concerning the surface terms, but moreover, the expressions for the primary and secondary first class constraints as well as their action on the field variables and their relation to the generators of coordinate transformations can be directly established from the general structure of the Noether currents.

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