Modified Hamiltonian formalism for higher-derivative theories

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Standard framework for dealing with higher-derivative theories is provided by Ostrogradski formalism. The main disadvantages of the Ostrogradski approach are:

- the Hamiltonian, being linear function of some momenta, is necessarily unbounded from below (this cannot be cured)
- the Ostrogradski Lagrangian leads to incorrect equations of motion.
- there is no straightforward transition from the Ostrogradski Lagrangian to the Hamiltonian formalism (the Legendre transformation cannot be performed).
An alternative approach.

- It leads directly to the Lagrangians which, gives correct equations of motion i.e.

\[
\sum_{k=0}^{n} (-1)^k \frac{d^k}{dt^k} \left( \frac{\partial L}{\partial q^{(k)}} \right) = 0 \quad (1)
\]

- no additional Lagrange multipliers are necessary
- for Lagrangians nonsingular in Ostrogradski sense the Legendre transformation takes the standard form.
First, let us recall Ostrogradski formulation. Let $L$ be of the form

$$L = L(q, \dot{q}, \ddot{q}, \ldots, q^{(n)}),$$

and we define new variables

$$q_1 = q, \quad q_2 = \dot{q}, \quad \ldots, \quad q_n = q^{(n-1)}. \quad (3)$$

Then $L$ takes the form

$$L = L(q_1, q_2, \ldots, q_n, \dot{q}_n),$$

and leads to incorrect equations of motion. Moreover, the canonical momenta provide the following primary constraints: $p_1 \approx 0, p_2 \approx 0, \ldots, p_{n-1} \approx 0.$
One deals with the latter problem by adding Lagrange multipliers enforcing the proper relation between new coordinates and time derivatives of the original ones \( q_i = q^{(i-1)} \)

\[
L \rightarrow L + \sum_{i=1}^{n-1} \lambda_i (\dot{q}_i - q_{i+1}).
\]  

(5)

The theory becomes constrained (in spite of the fact that the initial theory may be nonsingular in the Ostrogradski sense),

\[
\frac{\partial^2 L}{\partial \dot{q}_n^2} = \frac{\partial^2 L}{\partial q^{(n)^2}} \neq 0.
\]  

(6)
Then, using Dirac method for constrained systems, we obtain the Ostrogradski Hamiltonian:

\[ H = \sum_{i=1}^{n-1} p_i q_{i+1} + p_n q_n - L(q_1, \ldots, q_n, \dot{q}_n). \]  

(7)

The canonical equations following from \( H \) are equivalent to the initial Lagrangians ones.

Of course, the above Hamiltonian is not the Legendre transformation of Ostrogradski Lagrangian.
Ostrogradski approach

We have seen that the Ostrogradski approach is based on the idea that the consecutive time derivatives of the initial coordinate form new coordinates, \( q_i \sim q^{(i-1)} \).

However, it has been suggested by

- *H.J. Schmidt*, Phys. Rev. D49 (1994), 6345
- *S. Hawking, T. Hertog*, Phys. Rev. D65 (2002), 103515
- *T.-C. Cheng, P.-M. Ho, M.-C Yeh*, Phys. Rev. D65 (2002), 085015

that one can use every second derivative as a new variable,

\[ q_i \sim q^{(2i-2)}. \]  

(8)

We generalize this idea by introducing new coordinates as some functions of the initial ones and their time derivatives.
The case of even derivatives

Let us start with the Lagrangian with one degree of freedom depending on time derivatives up to some even order

\[ L = L(q, \dot{q}, \ldots, q^{(2n)}) , \tag{9} \]

and define new variables

\[ q_i = q^{(2i-2)}, \quad i = 1, \ldots, n+1, \]
\[ \dot{q}_i = q^{(2i-1)}, \quad i = 1, \ldots, n. \tag{10} \]

Then

\[ L = L(q_1, \dot{q}_1, q_2, \dot{q}_2, \ldots, q_n, \dot{q}_n, q_{n+1}). \tag{11} \]

Let further \( F \) be any function of the following variables

\[ F = F(q_1, \dot{q}_1, q_2, \dot{q}_2, \ldots, q_n, \dot{q}_n, q_{n+1}, q_{n+2}, \ldots, q_{2n}). \tag{12} \]

obeying

\[ \frac{\partial L}{\partial q_{n+1}} + \frac{\partial F}{\partial \dot{q}_n} = 0, \quad \text{det} \left[ \frac{\partial^2 F}{\partial q_i \partial \dot{q}_j} \right]_{\substack{n+2 \leq i \leq 2n \\ \text{for} \ 1 \leq j \leq n-1 \\ \text{not}}} \neq 0, \quad n \geq 2. \tag{13} \]
Finally, we define a new Lagrangian

\[ \mathcal{L} = L + \sum_{k=1}^{n} \left( \frac{\partial F}{\partial q_k} \dot{q}_k + \frac{\partial F}{\partial \dot{q}_k} q_{k+1} \right) + \sum_{j=n+1}^{2n} \frac{\partial F}{\partial q_j} \dot{q}_j. \] (14)

Let us have a look on Lagrange equations. For \( i = n + 1, \ldots, 2n \) we have

\[ \sum_{k=1}^{n} \frac{\partial^2 F}{\partial q_i \partial \dot{q}_k} (q_{k+1} - \ddot{q}_k) = 0, \quad i = n + 1, \ldots, 2n. \] (15)

By assumption about \( F \) one gets

\[ q_{k+1} = \ddot{q}_k, \quad k = 1, \ldots, n. \] (16)
Furthermore, from Lagrange equations for \( i = 1, \ldots, n \) we have

\[
\frac{\partial L}{\partial q_i} - \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}_i} \right) + \frac{\partial F}{\partial \dot{q}_i} - \frac{d^2}{dt^2} \left( \frac{\partial F}{\partial \dot{q}_i} \right) = 0, \quad i = 1, \ldots, n. \tag{17}
\]

By combining these equations and the definition of \( F \), one obtains

\[
\sum_{k=0}^{2n} (-1)^k \frac{d^k}{dt^k} \left( \frac{\partial L}{\partial q^{(k)}} \right) = 0. \tag{18}
\]

So, we arrive at the initial Lagrange equation.
Let us now consider the Hamiltonian formalism. The Legendre transformation can be immediately performed; neither additional Lagrange multipliers nor constraints analysis are necessary. One obtains

\[ p_i = \frac{\partial F}{\partial q_i}, \quad i = n + 1, \ldots, 2n, \tag{19} \]

\[ p_i = \frac{\partial L}{\partial \dot{q}_i} + \sum_{k=1}^{n} \left( \frac{\partial^2 F}{\partial \dot{q}_i \partial q_k} \dot{q}_k + \frac{\partial^2 F}{\partial \dot{q}_i \partial \dot{q}_k} \dot{q}_{k+1} \right) + \sum_{j=n+1}^{2n} \frac{\partial^2 F}{\partial \dot{q}_i \partial q_j} \dot{q}_j + \frac{\partial F}{\partial q_i}, \tag{20} \]

for \( i = 1, \ldots, n. \)

By the assumption about \( F, \) equations (19) can be solved for velocities

\[ \dot{q}_i = f_i(q_1, \ldots, q_{2n}, p_{n+1}, \ldots, p_{2n}), \quad i = 1, \ldots, n. \tag{21} \]
Now, eqs. (20) are linear with respect to $\dot{q}_i$ for $i = n + 1, \ldots, 2n$ and can be easily solved.

Finally, the Hamiltonian is calculated according to the standard prescription.

$$H = \sum_{i=1}^{2n} p_i \dot{q}_i - \mathcal{L} = \sum_{i=1}^{n} \left( p_i - \frac{\partial F}{\partial q_i} \right) \dot{q}_i - \sum_{i=1}^{n} \frac{\partial F}{\partial \dot{q}_i} \dot{q}_{i+1} - \mathcal{L}, \quad (22)$$

where everything is expressed in terms of $q$'s and $p$'s.
In order to compare the present formalism with the Ostrogradski approach let us define new (Ostrogradski) variables \( \tilde{q}_k, \tilde{p}_k, 1 \leq k \leq 2n \):

\[
\begin{align*}
\tilde{q}_{2i-1} &= q_i, \\
\tilde{q}_{2i} &= f_i(q_1, \ldots, q_{2n}, p_{n+1}, \ldots, p_{2n}), \\
\tilde{p}_{2i-1} &= p_i - \frac{\partial F}{\partial q_i}(q_1, f_1(\ldots), \ldots, q_n, f_n(\ldots), q_{n+1}, \ldots, q_{2n}), \\
\tilde{p}_{2i} &= -\frac{\partial F}{\partial f_i}(q_1, f_1(\ldots), \ldots, q_n, f_n(\ldots), q_{n+1}, \ldots, q_{2n}),
\end{align*}
\]

(23)

where \( i = 1, \ldots, n \) and \( f_i = \dot{q}_i \).

It is easily seen that the above transformation is a canonical one and the relevant generating function reads

\[
\Phi(q_1, \ldots, q_{2n}, \tilde{p}_1, \tilde{q}_2, \tilde{p}_3, \tilde{q}_4, \ldots, \tilde{p}_{2n-1}, \tilde{q}_{2n}) = \\
\sum_{k=1}^{n} q_k \tilde{p}_{2k-1} + F(q_1, \tilde{q}_2, q_2, \tilde{q}_4, \ldots, q_n, \tilde{q}_{2n}, q_{n+1}, \ldots, q_{2n}).
\]

(24)
The case of odd derivatives

Let us now consider the case of Lagrangian depending on time derivatives up to some odd order. Again, we define

\[ q_i = q^{(2i-2)}, \quad i = 1, \ldots, n + 1 \]
\[ \dot{q}_i = q^{(2i-1)}, \quad i = 1, \ldots, n + 1. \]  

(25)

Now, we select a function \( F \),

\[ F = F(q_1, \dot{q}_1, q_2, \dot{q}_2 \ldots, q_n, \dot{q}_n, q_{n+1}, q_{n+2}, \ldots, q_{2n+1}), \]  

(26)

subject to the single condition (let us note that no condition of the form (13) is here necessary),

\[ \det \left[ \frac{\partial^2 F}{\partial q_i \partial \dot{q}_j} \right]_{n+2 \leq i \leq 2n+1}^{1 \leq j \leq n} \neq 0, \]  

(27)

and define the Lagrangian

\[ \mathcal{L} = L + \sum_{k=1}^{n} \left( \frac{\partial F}{\partial q_k} \dot{q}_k + \frac{\partial F}{\partial \dot{q}_k} q_{k+1} \right) + \sum_{j=n+1}^{2n+1} \frac{\partial F}{\partial \dot{q}_j} \dot{q}_j. \]  

(28)
As before, the above Lagrangian gives the initial Lagrange equation. Similarly, we can perform the Legendre transformation obtaining

\[ H = \sum_{k=1}^{n+2} p_k \dot{q}_k - L - \sum_{k=1}^{n} \left( \frac{\partial F}{\partial q_k} \dot{q}_k + \frac{\partial F}{\partial \dot{q}_k} q_{k+1} \right) - \frac{\partial F}{\partial q_{n+1}} \dot{q}_{n+1}. \]  

(29)

Also this Hamiltonian is related to the Ostrogradski one by

\[
\begin{align*}
\tilde{q}_{2i-1} &= q_i, \\
\tilde{q}_{2j} &= f_j(q_1, \ldots, q_{2n+1}, p_{n+1}, \ldots, p_{2n+1}), \\
\tilde{p}_{2i-1} &= p_i - \frac{\partial F}{\partial q_i}(q_1, f_1(\ldots), \ldots, q_n, f_n(\ldots), q_{n+1}, \ldots, q_{2n+1}), \\
\tilde{p}_{2j} &= -\frac{\partial F}{\partial f_j}(q_1, f_1(\ldots), \ldots, q_n, f_n(\ldots), q_{n+1}, \ldots, q_{2n+1}),
\end{align*}
\]

where \( i = 1, \ldots, n+1, j = 1, \ldots, n \). The generating function reads

\[
\Phi(q_1, \ldots, q_{2n+1}, \tilde{p}_1, \tilde{q}_2, \tilde{p}_3, \tilde{q}_4, \ldots, \tilde{p}_{2n-1}, \tilde{q}_{2n}, \tilde{p}_{2n+1}) = \\
= \sum_{k=1}^{n+1} q_k \tilde{p}_{2k-1} + F(q_1, \tilde{q}_2, q_2, \tilde{q}_4, \ldots, q_n, \tilde{q}_{2n}, q_{n+1}, \ldots, q_{2n+1}).
\]  

(30)
Let us conclude this part with a simple example. Consider the Lagrangian

\[ L = \frac{1}{2} \dot{q}^2 - \frac{\omega^2}{2} q^2 - g q \ddot{q}^2 \]  \hspace{1cm} (31)

and define

\[ q_1 = q, \quad q_2 = \dot{q}. \]  \hspace{1cm} (32)

Let \( F \) be a function of the form

\[ F(q_1, \dot{q}_1, q_2) = 2g q_1 \dot{q}_1 q_2. \]  \hspace{1cm} (33)

Then new Lagrangian reads

\[ \mathcal{L} = \frac{1}{2} \dot{q}_1^2 - \frac{\omega^2}{2} q_1^2 + g q_1 q_2^2 + 2g \dot{q}_1^2 q_2 + 2g q_1 \dot{q}_1 \dot{q}_2. \]  \hspace{1cm} (34)
Example

It is now straightforward to construct the relevant Hamiltonian

\[ H = \frac{p_1 p_2}{2 g q_1} - \frac{(1 + 4 g q_2)}{8 g^2 q_1^2} p_2^2 + \frac{\omega^2}{2} q_1^2 - g q_1 q_2^2. \]  \hspace{1cm} (35)

The generating function to the Ostrogradski variables reads

\[ \Phi(q_1, q_2, \tilde{p}_1, \tilde{q}_2) = q_1 \tilde{p}_1 + 2 g q_1 q_2 \tilde{q}_2, \]  \hspace{1cm} (36)

and gives

\[ q_1 = \tilde{q}_1 \quad q_2 = -\frac{\tilde{p}_2}{2 g \tilde{q}_1} \]

\[ p_1 = \tilde{p}_1 - \frac{\tilde{p}_2 \tilde{q}_2}{\tilde{q}_1} \quad p_2 = 2 g \tilde{q}_1 \tilde{q}_2, \]

In terms of new variables we get the Ostrogradski Hamiltonian

\[ H = \tilde{p}_1 \tilde{q}_2 - \frac{\tilde{p}_2^2}{4 g \tilde{q}_1} - \frac{1}{2} \tilde{q}_2^2 + \frac{\omega^2}{2} \tilde{q}_1^2. \]  \hspace{1cm} (37)
The case of many degrees of freedom.

First, we will consider Lagrangians depending on first and second time derivatives. We expect that the counterpart of the condition (13) should be of the form

\[
\frac{\partial L}{\partial q_2^\mu} + \frac{\partial F}{\partial \dot{q}_1^\mu} = 0, \tag{38}
\]

but this condition is incorrect because the order in which we take partial derivatives is irrelevant. Therefore we must slightly modify our earlier considerations.
Let us start with Lagrangians containing time derivatives up to the second order

\[ L = L(q, \dot{q}, \ddot{q}), \quad (39) \]

here \( q = (q^\mu), \mu = 1, \ldots, N. \)

The nonsingularity condition of Ostrogradski reads

\[ \det \left( \frac{\partial^2 L}{\partial \ddot{q}^\mu \partial \ddot{q}^\nu} \right) \neq 0. \quad (40) \]

We define new coordinates \( q_1, \dot{q}_1, q_2 \)

\[ q^\mu = q_1^\mu, \quad \dot{q}^\mu = \dot{q}_1^\mu, \quad \ddot{q}^\mu = \chi^\mu(q_1, \dot{q}_1, q_2), \quad (41) \]

where \( \chi \) are the functions specified below.
First, we select a function, $F = F(q_1, \dot{q}_1, q_2)$, subject to the single condition

$$\det \left( \frac{\partial^2 F}{\partial \dot{q}_1^\mu \partial q_2^\nu} \right) \neq 0.$$  

(42)

Now, $\chi^\mu(q_1, \dot{q}_1, q_2)$ are defined as the unique (at least locally due to (40)) solution to the following set of equations:

$$\frac{\partial L(q_1, \dot{q}_1, \chi)}{\partial \chi^\mu} = - \frac{\partial F(q_1, \dot{q}_1, q_2)}{\partial \dot{q}_1^\mu}. $$  

(43)

The new Lagrangian is given by

$$\mathcal{L}(q_1, \dot{q}_1, q_2, \dot{q}_2) = L(q_1, \dot{q}_1, \chi(q_1, \dot{q}_1, q_2)) + \frac{\partial F(q_1, \dot{q}_1, q_2)}{\partial q_1^\mu} \dot{q}_1^\mu$$ $$+ \frac{\partial F(q_1, \dot{q}_1, q_2)}{\partial q_2^\mu} \dot{q}_2^\mu + \frac{\partial F(q_1, \dot{q}_1, q_2)}{\partial \dot{q}_1^\mu} \chi^\mu(q_1, \dot{q}_1, q_2).$$  

(44)
The equation of motion for $q_2^\mu$ yields

$$\frac{\partial^2 F}{\partial \dot{q}_1^\nu \partial q_2^\mu} (\chi^\nu - \ddot{q}_1^\nu) = 0; \quad (45)$$

which, by virtue of (42) implies, $\ddot{q}^\mu = \chi^\mu(q_1, \dot{q}_1, q_2)$. For the remaining variables $q_1^\mu$ one obtains

$$\frac{\partial L}{\partial q_1^\mu} - \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}_1^\mu} \right) + \frac{d^2}{dt^2} \left( \frac{\partial L}{\partial \chi^\mu} \right) = 0, \quad (46)$$

which together with the first equation gets the initial Lagrange equations.
One can also directly pass to the Hamiltonian picture:

\[
p_{2\mu} = \frac{\partial L}{\partial \dot{q}_{2}^\mu} = \frac{\partial F(q_{1}, \dot{q}_{1}, q_{2})}{\partial q_{2}^\mu} \tag{47}
\]

\[
p_{1\mu} = \frac{\partial L}{\partial \dot{q}_{1}^\mu} + \frac{\partial^{2} F}{\partial q_{1}^\nu \partial \dot{q}_{1}^\mu} \dot{q}_{1}^\nu + \frac{\partial^{2} F}{\partial \dot{q}_{1}^\mu \partial \dot{q}_{1}^\nu} \chi^\nu + \frac{\partial^{2} F}{\partial \dot{q}_{1}^\mu \partial q_{2}^\nu} \dot{q}_{2}^\nu + \frac{\partial F}{\partial q_{1}^\mu}. \tag{48}
\]

Using (42) the first set of equations can be solved for \( \dot{q}_{1}^\mu \) and then the second set is linear in terms of \( \dot{q}_{2}^\mu \). So, we get \( \dot{q}_{2}^\mu \).

The Hamiltonian \( H \) is computed in standard way:

\[
H = p_{1\mu} \dot{q}_{1}^\mu - L - \frac{\partial F}{\partial q_{1}^\mu} \dot{q}_{1}^\mu - \frac{\partial F}{\partial \dot{q}_{1}^\mu} \chi^\mu, \tag{49}
\]

where everything is expressed in terms of \( q_{1}, q_{2}, p_{1}, p_{2} \).
One can check, by direct calculation, that the canonical equations following from $H$ are equivalent to the initial Lagrangians ones.

There exists canonical transformation which relates our Hamiltonian to the Ostrogradski one. It reads

$$
\tilde{q}_1^\mu = q_1^\mu,
\tilde{q}_2^\mu = f^\mu(q_1, q_2, p_2),
\tilde{p}_{1\mu} = p_{1\mu} - \frac{\partial F}{\partial q_1^\mu}(q_1, f, q_2),
\tilde{p}_{2\mu} = -\frac{\partial F}{\partial f^\mu}(q_1, f, q_2),
$$

(50)

where tilde refers to Ostrogradski variables and $f^\mu = \dot{q}_1^\mu$. 
Let us consider a nonsingular Lagrangian of the form

\[ L = L(q, \dot{q}, \ddot{q}). \] (51)

It is slightly surprising that this case (and, in general, the case when the highest time derivatives are of odd order) is simpler.

We define the new variables \( q_1, \dot{q}_1, q_2, \dot{q}_2 \)

\[ q^{\mu} = q_1^{\mu}, \quad \dot{q}^{\mu} = \dot{q}_1^{\mu}, \quad \ddot{q}^{\mu} = q_2^{\mu}, \quad \dddot{q}^{\mu} = \dot{q}_2^{\mu}. \] (52)
Let $F$ be a function such that

$$F = F(q_1, \dot{q}_1, q_2, q_3), \quad \det \left( \frac{\partial^2 F}{\partial \dot{q}_1^\mu \partial q_3^\nu} \right) \neq 0. \quad (53)$$

The modified Lagrangian reads

$$\mathcal{L} = L + \frac{\partial F}{\partial q_1^\mu} \dot{q}_1^\mu + \frac{\partial F}{\partial q_2^\mu} \dot{q}_2^\mu + \frac{\partial F}{\partial q_3^\mu} \dot{q}_3^\mu + \frac{\partial F}{\partial \dot{q}_1^\mu} q_2^\mu, \quad (54)$$

and it gives Lagrange equations for the initial variables for the original variable.
The case of third derivatives

As in the second-order case, the Legendre transformation can be directly performed and Hamiltonian is of the form

\[
H = p_{1\mu} \dot{q}_1^\mu + p_{2\mu} \dot{q}_2^\mu - L - \frac{\partial F}{\partial q_1^\mu} \dot{q}_1^\mu - \frac{\partial F}{\partial \dot{q}_1^\mu} q_2^\mu - \frac{\partial F}{\partial q_2^\mu} \dot{q}_2^\mu. \tag{55}
\]

The canonical transformation which relates our formalism to the Ostrogradski is of the form

\[
\tilde{q}_1^\mu = q_1^\mu, \quad \tilde{q}_3^\mu = q_2^\mu, \\
\tilde{q}_2^\mu = f^\mu(q_1, q_2, q_3, p_3), \\
\tilde{p}_{1\mu} = p_{1\mu} - \frac{\partial F}{\partial q_1^\mu}(q_1, f(q_1, q_2, q_3, p_3), q_2, q_3), \\
\tilde{p}_{3\mu} = p_{2\mu} - \frac{\partial F}{\partial q_2^\mu}(q_1, f(q_1, q_2, q_3, p_3), q_2, q_3), \\
\tilde{p}_{2\mu} = - \frac{\partial F}{\partial \dot{f}^\mu}(q_1, f(q_1, q_2, q_3, p_3), q_2, q_3), \tag{56}
\]

where \( f^\mu = \dot{q}_1^\mu \).
Presented approach is also applicable to singular Lagrangians and the results agree with the conclusions for Ostrogradski formalism and possess generalization to the case of field theory.

More detailed discussion and references:
"Modified Hamiltonian formalism for higher-derivative theories", Physical Review D 82 2010, 045008

For example if we consider formulation of $f(R)$ gravity with the metric of the form

$$ds^2 = -N^2 dt^2 + a^2 d\vec{x}^2.$$  \hfill (57)
Then the curvature of the metric reads

$$R = 6\left(\frac{\dot{a}}{NA}\right) + 12\left(\frac{\dot{a}}{Na}\right)^2 \quad (58)$$

and the Lagrangian of $f(R)$ gravity takes the form

$$L(a, N) = \frac{1}{2} Na^3 f(R). \quad (59)$$

In our case the curvature $R$ can be one of the basic variables

$$a_1 = a, \quad \dot{a}_1 = \dot{a}, \quad N_1 = N, \quad \dot{N}_1 = \dot{N}, \quad a_2 = R. \quad (60)$$
Thank you for your attention