Hamiltonian structure of scalar-tensor theories beyond Horndeski

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Received August 12, 2014
Accepted September 22, 2014
Published October 27, 2014

Abstract. We study the nature of constraints and the Hamiltonian structure in a scalar-tensor theory of gravity recently proposed by Gleyzes, Langlois, Piazza and Vernizzi (GLPV). For the simple case with $A_5 = 0$, namely when the canonical momenta conjugate to the spatial metric are linear in the extrinsic curvature, we prove that the number of physical degrees of freedom is three at fully nonlinear level, as claimed by GLPV. Therefore, while this theory extends Horndeski’s scalar-tensor gravity theory, it is protected against additional degrees of freedom.

Keywords: modified gravity, gravity

ArXiv ePrint: 1408.0670
1 Introduction

Mysteries in modern cosmology such as inflation, dark energy and dark matter have been strong motivations for alternative gravity theories beyond Einstein’s general relativity, both in the UV and in the IR. Because of Lovelock’s theorem \cite{1,2}, modification of general relativity requires inclusion of at least one of the following: (i) extra degrees of freedom, (ii) extra dimensions, (iii) higher derivative terms, (iv) extension of (pseudo-)Riemannian geometry, (v) non-locality. Scalar-tensor theories of gravity are examples of the type (i).

The most general scalar-tensor theory with three degrees of freedom and second-order equations of motion was found in 1974 by Horndeski \cite{3} and rediscovered recently in the context of the so-called Galileon theory \cite{4–6}. In this theory, while each term in the action can in general include more than two derivatives, the equations of motion are independent of derivatives higher than second-order. This is achieved by special choice of coupling constants.

In the context of low-energy effective field theories, one should include all possible terms that are consistent with symmetries and then truncate the infinite series of terms according to the standard derivative expansion and power-counting. In this language, Horndeski’s theory is rather fine-tuned. Such fine-tuning is expected to be detuned by quantum loops in general.

It is thus of theoretical interest to see what the number of physical degrees of freedom is in detuned theories. Generic deviation from the fine-tuning invoked by Horndeski’s theory would introduce extra degrees of freedom, at least formally. If such deviation is small enough then frequencies or momenta of those extra degrees of freedom are higher than the cutoff scale of the theory and we can safely integrate them out. The theory then remains healthy in the domain of its validity as a low energy effective theory. In this case, although the theory formally (or apparently) includes extra degrees of freedom, they are usually considered unphysical and not included in the physical spectrum of the theory.

In a recent paper \cite{7}, Gleyzes, Langlois, Piazza and Vernizzi (GLPV) asked a similar but slightly different question: they asked whether it is possible to extend Horndeski’s theory without introducing extra degrees of freedom even formally, irrespective of whether they are in the regime of validity of the low energy effective theory or not. Considering our complete ignorance of the nature of dark energy, we consider this as a legitimate attitude. GLPV
then proposed a class of scalar-tensor theories of gravity that extends Horndeski’s theory and claimed that the number of degrees of freedom in this class of theories remains the same as in Horndeski’s theory, i.e. three, at a fully nonlinear level. However, as we shall see later, their analysis is not complete: what is called the momentum constraint in \[7\] lacks a contribution from the scalar degree of freedom hidden in the lapse function and, as a result, is not first-class. The purpose of the present paper is to count the number of degrees of freedom in the GLPV theory by performing Hamiltonian analysis properly.

The rest of the paper is organized as follows. In section 2 we briefly describe the action of the GLPV theory in the unitary gauge, adopting the ADM decomposition. In section 3 we find the complete set of primary and secondary constraints for the system and divide them into the set of first-class constraints and that of second-class constraints. In section 4, adding gauge-fixing conditions, we end up with 14 second-class constraints in the 20-dimensional phase space and thus conclude that the number of degrees of freedom is three, as claimed by GLPV. Section 5 is devoted to a summary and discussions. In appendix A, we summarize the Hamiltonian canonical formulation and the treatment of constraints. Appendix B outlines the calculations of Poisson brackets.

2 Unitary gauge action

As far as the derivative of a scalar field \(\partial_\mu \phi\) is timelike, one can choose the time coordinate \(t\) so that

\[
\phi = t. \tag{2.1}
\]

This choice of time coordinate is often called unitary gauge. By adopting the ADM decomposition

\[
ds^2 = -N^2 dt^2 + h_{ij}(dx^i + N^i dt)(dx^j + N^j dt), \tag{2.2}
\]

the action of the GLPV theory in the unitary gauge is [7]

\[
S = \int d^3 x dt N \sqrt{h} \sum_{n=2}^{5} L_n, \tag{2.3}
\]

where

\[
L_2 = A_2(t, N),
L_3 = A_3(t, N) K, \\
L_4 = A_4(t, N) K_2 + B_4(t, N) R, \\
L_5 = A_5(t, N) K_3 + B_5(t, N) K^{ij} G_{ij},
\]

and

\[
K = K^{i}_i, \\
K_2 = K^2 - K^i_j K^j_i, \\
K_3 = K^3 - 3 K K^{ij} K_{ij} + 2 K^i_j K^j_k K^k_i. \tag{2.5}
\]

Here, \(R\) and \(G_{ij}\) are the Ricci scalar and the Einstein tensor of the 3-dimensional spatial metric \(h_{ij}\),

\[
K_{ij} = \frac{1}{2N} (\partial_i h_{ij} - D_i N_j - D_j N_i) \tag{2.6}
\]

\[1\]For phenomenological applications, see [7, 11–16].
is the extrinsic curvature, and the spatial indices are lowered and raised by \( h_{ij} \) and its inverse \( h^{ij} \).

### 3 Nature of constraints

The action does not include time derivatives of \( N^i \) and \( N \), and thus we have the primary constraints

$$
\pi_i = 0, \quad \pi_N = 0,
$$

where \( \pi_N \) and \( \pi_i \) are canonical momenta conjugate to \( N \) and \( N^i \), respectively. The canonical momentum conjugate to \( h_{ij} \) is

$$
\pi^{ij} = \frac{\sqrt{h}}{2} \left\{ A_3 h^{ij} + 2A_4 (h^{ij} K - K^{ij}) + 3A_5 \left[ h^{ij} (K^2 - K^k_i K^l_k) + 2(K^k_i K^kj - K K^{ij}) \right] + B_5 G^{ij} \right\}.
$$

The Hamiltonian is then given by

$$
H = \int d^3 x \left( \pi^{ij} \partial_t h_{ij} - N \sqrt{h} \sum_{n=2}^5 L_n + \lambda^i \pi_i + \lambda_N \pi_N \right),
$$

where \( \lambda_N \) and \( \lambda^i \) are Lagrange multipliers associated with the primary constraints (3.1). We define the Poisson bracket as usual by

$$
\{ F, G \}_P \equiv \int d^3 x \left[ \frac{\delta F}{\delta N(x)} \frac{\delta G}{\delta \pi_N(x)} + \frac{\delta F}{\delta N^i(x)} \frac{\delta G}{\delta \pi_i(x)} + \frac{\delta F}{\delta h_{ij}(x)} \frac{\delta G}{\delta \pi^{ij}(x)} - \frac{\delta F}{\delta \pi^{ij}(x)} \frac{\delta G}{\delta h_{ij}(x)} \right].
$$

Since the shift vector \( N^i \) enters (3.2) only implicitly though the extrinsic curvature \( K_{ij} \), we have

$$
\frac{\delta H}{\delta N^i} \bigg|_{N,h_{ij},\pi_N,\pi_i,\pi^{ij},\lambda_N,\lambda^i} = \frac{\delta H}{\delta N^j} \bigg|_{N,h_{ij},\pi_N,\pi_i,K_{ij},\lambda_N,\lambda^i} = -2\sqrt{h} D_j \left( \frac{\pi^j}{\sqrt{h}} \right),
$$

provided that (3.2) can be solved with respect to \( K_{ij} \). Here, the l.h.s. is the partial functional derivative of \( H \), considered as a \( t \)-dependent functional of \( (N, N^i, h_{ij}, \pi_N, \pi_i, \pi^{ij}, \lambda_N, \lambda^i) \), with respect to \( N^i \). The second expression is the partial functional derivative of \( H \), considered as a \( t \)-dependent functional of \( (N, N^i, h_{ij}, \pi_N, \pi_i, K_{ij}, \lambda_N, \lambda^i) \), with respect to \( N^j \). Hence, the Hamiltonian is of the following form,

$$
H = \int d^3 x \left( \mathcal{H} + N^i \mathcal{H}_i + \lambda_N \pi_N + \lambda^i \pi_i \right),
$$

where

$$
\mathcal{H}_i \equiv -2\sqrt{h} D_j \left( \frac{\pi^j}{\sqrt{h}} \right),
$$

and

$$
\mathcal{H} = \mathcal{H}(t, N, h_{ij}, \pi^{kl})
$$
depends only on \((t, N, h_{ij}, \pi^{jk})\). Here, \(D_j\) is the 3-dimensional covariant derivative compatible with the spatial metric \(h_{ij}\).

From now on, we set \(A_5 = 0\) for simplicity. With \(A_5 = 0\), the canonical momentum conjugate to \(h_{ij}\) is

\[
\pi^{ij} = \frac{\sqrt{h}}{2} \left[ A_3 h^{ij} + 2 A_4 (h^{ij} K - K^{ij}) + B_5 G^{ij} \right]. \tag{3.9}
\]

Provided that \(A_4 \neq 0\), this relation is equivalent to

\[
K_{ij} = - \frac{1}{A_4} \left[ \frac{1}{\sqrt{h}} \left( \pi_{ij} - \frac{1}{2} h_{ij} \pi \right) + \frac{A_3 \pi}{2 \sqrt{h} A_4} - \frac{3 A_3}{8 A_4} + B_5 R + \frac{B_5}{4 A_4} \left( R_{ij} - \frac{3}{8} R \right) \right]. \tag{3.10}
\]

where \(\pi \equiv h_{ij} \pi^{ij}\) and \(R_{ij}\) is the Ricci tensor of \(h_{ij}\). Hence, as far as \(A_4 \neq 0\), i.e. as far as the graviton has a non-vanishing kinetic term, there is no additional primary constraint other than (3.1). The Hamiltonian is of the form (3.6)–(3.7) with

\[
\mathcal{H} = - N \sqrt{h} \left[ \frac{1}{A_4} \left( \frac{\pi_{ij} \pi^{ij}}{h} - \frac{\pi^2}{2h} \right) + \frac{A_3 \pi}{2 \sqrt{h} A_4} - \frac{3 A_3}{8 A_4} + A_2 + B_4 R \right.

\[\left. - \frac{B_5}{A_4 \sqrt{h}} \left( \pi_{ij} R_{ij} - \frac{1}{4} \pi R \right) + \frac{A_3 B_5}{8 A_4} R + \frac{B_5^2}{4 A_4} \left( R_{ij} R_{ij} - \frac{3}{8} R^2 \right) \right]. \tag{3.11}
\]

Hereafter, we consider \(\mathcal{H}\) as a function of \((t, N, h_{ij}, \pi^{ij})\).

We have the primary constraints (3.1). Since\(^2\)

\[
\frac{d}{dt} \pi_i(x) \approx \{\pi_i(x), \mathcal{H}\}_P = - \mathcal{H}_i - \int d^3 y \left[ \frac{\delta \mathcal{L}^i(y)}{\delta N^i(x)} \pi_j(y) + \frac{\delta \mathcal{L}^N(y)}{\delta N(x)} \pi_j(y) \right] \approx - \mathcal{H}_i,
\]

\[
\frac{d}{dt} \pi_N(x) \approx \{\pi_N(x), \mathcal{H}\}_P = - \frac{\partial \mathcal{H}}{\partial N} - \int d^3 y \left[ \frac{\delta \mathcal{L}^i(y)}{\delta N^i(x)} \pi_j(y) + \frac{\delta \mathcal{L}^N(y)}{\delta N(x)} \pi_j(y) \right] \approx - \frac{\partial \mathcal{H}}{\partial N}, \tag{3.12}
\]

the corresponding secondary constraints are

\[
\mathcal{H}_i \approx 0, \quad C \approx 0, \tag{3.13}
\]

where \(\approx\) denotes an equality in the weak sense, i.e. the equality holds once the constraints are imposed, and we have defined

\[
C \equiv - \frac{\partial \mathcal{H}}{\partial N}
\]

\[
= \sqrt{h} \left[ \left( \frac{\pi_{ij} \pi^{ij}}{h} - \frac{\pi^2}{2h} \right) \frac{\partial}{\partial N} \left( \frac{N A_3}{A_4} \right) + \frac{\pi}{2 \sqrt{h}} \frac{\partial}{\partial N} \left( \frac{N A_3}{A_4} \right) - \frac{3}{8} \frac{\partial}{\partial N} \left( \frac{N A_3}{A_4} \right) + \frac{\partial (N A_2)}{\partial N} + R \frac{\partial (N B_4)}{\partial N} \right.

\[\left. - \frac{1}{\sqrt{h}} \left( \pi_{ij} R_{ij} - \frac{1}{4} \pi R \right) \right) \frac{\partial}{\partial N} \left( \frac{N B_5}{A_4} \right) + R \frac{\partial}{\partial N} \left( \frac{N A_3 B_5}{8 A_4} \right) + \left( R_{ij} R_{ij} - \frac{3}{8} R^2 \right) \frac{\partial}{\partial N} \left( \frac{N B_5^2}{4 A_4} \right) \right]. \tag{3.14}
\]

\(\text{\textsuperscript{2}}\)The first equality in each of the following two equations is weak one since the Lagrange multipliers in the Hamiltonian may depend on canonical variables. See (A.7) for this point. A similar remark applies to the first equality in each equation in (3.24) and (3.28) below.
Since $A_{2,3,4}$ and $B_{4,5}$ depend on $N$, $C$ generically depends on $N$. The constraint $C \approx 0$ then determines $N$ if

$$\frac{\partial^2 \mathcal{H}}{\partial N^2} \neq 0.$$  \hspace{1cm} (3.15)

It is straightforward to show that $^3$

$$\{ \bar{\mathcal{H}}[f], \bar{\mathcal{H}}[g] \}_P \approx \bar{\mathcal{H}}[[f, g]] \approx 0, \quad \text{for } \forall f^i, \forall g^i,$$  \hspace{1cm} (3.16)

where we have defined

$$\bar{\mathcal{H}}[f] \equiv \int d^3x f^i(x) \mathcal{H}_i(x), \quad [f, g] \equiv f^j \partial_j g^i - g^j \partial_j f^i.$$  \hspace{1cm} (3.17)

However, under the condition (3.15), the Poisson bracket between $\mathcal{H}_i(x)$ and $C(y)$ fails to vanish weakly as

$$\{ \bar{\mathcal{H}}[f], \bar{C}[\varphi] \}_P \approx \bar{C}[f \partial \varphi] - \int d^3x \frac{\partial^2 \mathcal{H}}{\partial N^2} f^i \partial_i N \approx - \int d^3x \frac{\partial^2 \mathcal{H}}{\partial N^2} f^i \partial_i N,$$  \hspace{1cm} \text{for } \forall f^i, \forall \varphi, (3.18)

where we have defined

$$\bar{C}[\varphi] \equiv \int d^3x \varphi(x) C(x), \quad f \partial \varphi \equiv f^i \partial_i \varphi.$$  \hspace{1cm} (3.19)

Therefore, contrary to what was claimed by GLPV [7], the constraint $\mathcal{H}_i \approx 0$ is not first-class.

Nonetheless, defining the following linear combination of constraints

$$\mathcal{H}_i^{\text{tot}} = \mathcal{H}_i + \pi_N \partial_i N,$$  \hspace{1cm} (3.20)

it is possible to show that

$$\{ \bar{\mathcal{H}}^{\text{tot}}[f], \bar{\pi}_N[\varphi] \}_P \approx \bar{\pi}_N[f \partial \varphi] \approx 0, \quad \{ \bar{\mathcal{H}}^{\text{tot}}[f], \bar{C}[\varphi] \}_P \approx \bar{C}[f \partial \varphi] \approx 0, \quad \{ \bar{\mathcal{H}}^{\text{tot}}[f], \bar{\mathcal{H}}^{\text{tot}}[g] \}_P \approx \bar{\mathcal{H}}^{\text{tot}}[[f, g]] \approx 0, \quad \text{for } \forall f^i, \forall g^i, \forall \varphi,$$  \hspace{1cm} (3.21)

where we have defined

$$\bar{\mathcal{H}}^{\text{tot}}[f] \equiv \int d^3x f^i(x) \mathcal{H}_i^{\text{tot}}(x), \quad \bar{\pi}_N[\varphi] \equiv \int d^3x \varphi(x) \pi_N(x).$$  \hspace{1cm} (3.22)

By definition we also have

$$\{ \pi_i(x), \pi_j(y) \}_P = 0, \quad \{ \pi_i(x), \pi_N(y) \}_P = 0, \quad \{ \pi_i(x), C(y) \}_P = 0, \quad \{ \pi_i(x), \mathcal{H}_j^{\text{tot}}(y) \}_P = 0.$$  \hspace{1cm} (3.23)

Furthermore,

$$\frac{d}{dt} \bar{\mathcal{H}}^{\text{tot}}[f] \approx \{ \bar{\mathcal{H}}^{\text{tot}}[f], H \}_P \approx \bar{\mathcal{H}}[[f, N]] + \bar{\pi}_N[f \partial \lambda_N] \approx 0.$$  \hspace{1cm} (3.24)

$^3$The first equality below is kept weak just in case $f^i$ and/or $g^i$ may depend on canonical variables, and it becomes strong one if both $f^i$ and $g^i$ are independent of them. A similar remark applies to the first equality in each equation in (3.18) and (3.21) and the second equality in (3.24) below.
Therefore, it is concluded that constraints $\pi_i \approx 0$ and $H_i^{\text{tot}} \approx 0$ ($i = 1, 2, 3$) are first-class and that there is no additional secondary constraint associated with them.

It is easy to show that

$$\{\pi_N(x), \pi_N(y)\}_P = 0,$$

$$\{C(x), \pi_N(y)\}_P = -\frac{\partial^2 H}{\partial N^2} \delta^3(x - y).$$

Hence, provided that the condition (3.15) is satisfied, the determinant

$$\det \left( \begin{array}{cc}
\{\pi_N(x), \pi_N(y)\}_P & \pi_N(x), \pi_N(y)\}_P \\
\{C(x), \pi_N(y)\}_P & \{C(x), \pi_N(y)\}_P 
\end{array} \right)$$

(3.26)

does not vanish weakly, meaning that the set of constraints $\pi_N \approx 0$ and $C \approx 0$ is second-class.

The total Hamiltonian is

$$H_{\text{tot}} = \int d^3x \left[ H + N^i H_i + n^i H_i^{\text{tot}} + \lambda^i \pi_i + \lambda_N \pi_N + \lambda_C C \right]$$

$$= \int d^3x \left[ H + (N^i + n^i) H_i + \lambda^i \pi_i + (\lambda_N + n^i \partial_i N) \pi_N + \lambda_C C \right],$$

(3.27)

where $n^i$ and $\lambda_C$ are Lagrange multipliers. Since the set of constraints $\pi_N \approx 0$ and $C \approx 0$ is second-class, the consistency conditions,

$$\frac{d}{dt} \pi_N(x) \approx \{\pi_N(x), H_{\text{tot}}\}_P \approx 0, \quad \frac{d}{dt} C(x) \approx \partial_t \{C(x), H_{\text{tot}}\}_P \approx 0,$$

(3.28)

determine the two Lagrange multipliers $\lambda_N$ and $\lambda_C$, instead of generating additional secondary constraints.

4 Number of degrees of freedom

One can fix the gauge freedom associated with the first-class constraints $\pi_i \approx 0$ and $H_i^{\text{tot}} \approx 0$ by imposing additional conditions

$$G^i(x) \approx 0, \quad F^i(x) \approx 0, \quad (i = 1, 2, 3),$$

(4.1)

provided that the determinant

$$\det \left( \begin{array}{cc}
\frac{\delta G^i(y)}{\delta N^i(x)} & \frac{\delta F^i(y)}{\delta N^i(x)} \\
\frac{\delta G^j(y)}{\delta N^j(x)} & \frac{\delta F^j(y)}{\delta N^j(x)} 
\end{array} \right)$$

(4.2)

does not vanish weakly. Including the gauge fixing conditions, we thus have the following set of 14 second-class constraints:

$$H_i^{\text{tot}} \approx 0, \quad \pi_i \approx 0, \quad G^i(x) \approx 0, \quad F^i(x) \approx 0, \quad \pi_N \approx 0, \quad C \approx 0, \quad (i = 1, 2, 3).$$

(4.3)

The total Hamiltonian after gauge fixing is thus

$$H'_{\text{tot}} = \int d^3x \left[ H + N^i H_i + n^i H_i^{\text{tot}} + \lambda^i \pi_i + \lambda^i G^i + \lambda^i F^i + \lambda_N \pi_N + \lambda_C C \right]$$

$$= \int d^3x \left[ H + (N^i + n^i) H_i + \lambda^i \pi_i + \lambda^i G^i + \lambda^i F^i + (\lambda_N + n^i \partial_i N) \pi_N + \lambda_C C \right],$$

(4.4)
where $\lambda^G_i$ and $\lambda^F_i$ are Lagrange multipliers. As usual with the second-class constraints, the set of all Lagrange multipliers ($n^i, \lambda^i, \lambda^G_i, \lambda^F_i, \lambda_N, \lambda_C$) are fully determined by imposing

$$\{H_i(x), H'_\text{tot}(x)\}_P \approx 0, \quad \{\pi_i(x), H'_\text{tot}(x)\}_P \approx 0, \quad \frac{\partial}{\partial t} G^i(x) + \{G^i(x), H'_\text{tot}(x)\}_P \approx 0, \quad \frac{\partial}{\partial t} F^i(x) + \{F^i(x), H'_\text{tot}(x)\}_P \approx 0, \quad \frac{\partial}{\partial t} \pi_N(x) + \{\pi_N(x), H'_\text{tot}(x)\}_P \approx 0, \quad \frac{\partial}{\partial t} \pi_{ij}(x) + \{\pi_{ij}(x), H'_\text{tot}(x)\}_P \approx 0.$$  

(4.5)

Hence, starting with the 20-dimensional phase space ($N, N^i, h_{ij}, \pi_N, \pi_{ij}$), we end up with 6-dimensional physical phase space after imposing the 14 second-class constraints (4.3). Therefore, the number of degrees of freedom is three, as claimed by GLPV.

As a simple example of the gauge fixing functions, let us consider

$$G^i = N^i, \quad F^i = F^i(N, h_{ij}, \pi_N, \pi_{ij}; t),$$  

(4.6)

such that the determinant

$$\det \left( \{H'_\text{tot}(x), F^j(y)\}_P \right)$$  

(4.7)

does not vanish weakly. In this case the consistency conditions

$$\frac{dG^i}{dt} \approx 0, \quad \frac{d\pi_i}{dt} \approx 0,$$  

(4.8)

determine the six Lagrange multipliers $\lambda^i$ and $\lambda^G_i$ as

$$\lambda^i = 0, \quad \lambda^G_i = -H^i.$$  

(4.9)

By substituting them, we obtain

$$H'_\text{tot} = \int d^3x \left[ H + n^i H'_\text{tot}^i + \lambda^F_i F^i + \lambda_N \pi_N + \lambda_C C \right].$$  

(4.10)

Together with the gauge fixing condition $G^i = N^i \approx 0$, we see that the canonical pair ($N^i, \pi_i$) is fully eliminated from the phase space. The dimension of the reduced phase space ($N, h_{ij}, \pi_N, \pi_{ij}$) is 14. As usual with the second-class constraints, the set of all remaining Lagrange multipliers ($n^i, \lambda^F_i, \lambda_N, \lambda_C$) are fully determined by imposing

$$\{H'_\text{tot}(x), H'_\text{tot}(x)\}_P \approx 0, \quad \frac{\partial}{\partial t} F^i(x) + \{F^i(x), H'_\text{tot}(x)\}_P \approx 0, \quad \{\pi_N(x), H'_\text{tot}(x)\}_P \approx 0, \quad \frac{\partial}{\partial t} \pi_N(x) + \{\pi_N(x), H'_\text{tot}(x)\}_P \approx 0, \quad \frac{\partial}{\partial t} C(x) + \{C(x), H'_\text{tot}(x)\}_P \approx 0.$$  

(4.11)

There remains the following set of 8 second-class constraints acted on the 14-dimensional reduced phase space:

$$H'_\text{tot}^i \approx 0, \quad F^i(x) \approx 0, \quad \pi_N \approx 0, \quad C \approx 0, \quad (i = 1, 2, 3).$$  

(4.12)

Hence, we end up with 6-dimensional physical phase space, and the number of degrees of freedom is three.
5 Summary and discussions

We have investigated the nature of constraints and the Hamiltonian structure in the scalar-tensor theory recently proposed by Gleyzes, Langlois, Piazza and Vernizzi (GLPV) [7]. For the simple case with $A_5 = 0$, we have proved that the number of independent degrees of freedom is three at fully nonlinear level, as claimed by GLPV.

The Hamiltonian analysis in the present paper is similar to but actually differs from that done by GLPV for a couple of reasons. First, in the present paper the momentum constraint, that is the generator of the spatial diffeomorphism, is given by (3.20). Compared with the corresponding expression by GLPV, this includes an additional term of the form $\pi_N \partial_i N$, where $N$ is the lapse function and $\pi_N$ is the canonical momentum conjugate to $N$. The presence of the additional term of this form is expected from physical viewpoints: the time-space component of the stress-energy tensor of a scalar field should contribute to the total momentum constraint but the scalar field is encoded in the lapse function in the unitary gauge. Indeed, without the additional term, the Poisson bracket between the momentum constraint and the other secondary constraint $C$ would not vanish weakly, and thus the momentum constraint would not be first-class. Second, in the present paper we include not only $A_{2,3,4}$ and $B_4$ but also $B_5$. In spite of these differences, our analysis still supports the claim by GLPV: the number of degrees of freedom is three.

It is expected that inclusion of $A_5 \neq 0$ and more general terms [8] does not change the constraint algebra and thus the number of degrees of freedom. However, the analysis becomes technically involved and thus we consider it as beyond the scope of the present paper.

The Hamiltonian analysis in the present paper is based on the unitary gauge, in which the scalar field is encoded in the lapse function (and the time variable). Extension of the analysis to a general gauge is also beyond the scope of the present paper but we would like to make some comments on it here. It should be possible to obtain canonical transformation that maps the set of phase space variables in the unitary gauge to that in a general gauge. The constraints among the phase space variables in the unitary gauge, which we analyzed in the present paper, are then transformed to those in the general gauge. The algebra of constraints should be the same in any gauge. Together with the first-class constraint corresponding to the time diffeomorphism, it should be possible to show that the dimension of the physical phase space is six and that the number of degrees of freedom is three. However, we shall leave this analysis to a future work.

Acknowledgments

This work was supported in part by WPI Initiative, MEXT, Japan, Grant-in-Aid for Scientific Research 24540256 and Grant-in-Aid for JSPS Fellows. We would like to thank N. Tanahashi for useful discussions.

A Hamiltonian analysis of constrained system

In this appendix, we summarize the standard Hamiltonian analysis of a system with constraints.\textsuperscript{4} The standard analysis was introduced by P. Dirac in 50s and 60s [9, 10], as a way of quantizing mechanical systems such as gauge theories.

\textsuperscript{4}In this appendix, we consider a finite number of coordinate variables $q_I$ for simplicity. If we extend this formalism to a (bosonic) field theory, we consider field variables instead and perform the procedure in a similar manner, as we have done in the main text. In this case, however, the coordinate indices $I$ and $J$ in (A.1)
We consider a system which has the following action,

\[ S = \int dt \, L(q^I, \dot{q}^J, t), \quad I, J = 1, 2, \ldots, N, \]  

(A.1)

where \(q^I\) are Grassmann even coordinate variables and an overdot denotes a derivative with respect to time \(t\). The Lagrangian \(L\) may depend on time explicitly. The canonical momentum \(p^I\) and the Hamiltonian \(\tilde{H}\) are defined as

\[ p^I \equiv \frac{\partial L}{\partial \dot{q}^I}, \]  

(A.2)

\[ \tilde{H} \equiv p^I \dot{q}^I - L. \]  

(A.3)

In the cases where the system is singular, (A.2) cannot completely be solved for \(\dot{q}^I\); this happens when

\[ \det \left| \frac{\partial^2 L}{\partial \dot{q}^I \partial \dot{q}^J} \right| = 0. \]  

(A.4)

Eq. (A.4) means that we have \(M_1 = N - r_0\) constraints independent from \(\dot{q}^I\), where \(r_0 = \text{rank}(\partial^2 L/\partial \dot{q}^I \partial \dot{q}^J)\). We denote these “primary” constraints as

\[ \phi_A(q^I, p^J, t) = 0, \quad A = 1, 2, \ldots, M_1. \]  

(A.5)

Including the information of the constraints into the Hamiltonian, we define a new Hamiltonian

\[ H = \tilde{H} + \phi_A \lambda^A. \]  

(A.6)

where \(\lambda^A\) are Lagrange multipliers. The inclusion of \(\phi_A \lambda^A\) should not be considered artificial; it merely represents the degree of arbitrariness proportional to \(\phi_A\) in defining the Hamiltonian from the Lagrangian. Thus \(\tilde{H}\) and \(H\) cannot be physically distinguished on the surface defined by \(\phi_A = 0\).

For an arbitrary function \(F(q^I, p^J, t)\), we can find its time evolution using the canonical equations by

\[ \frac{d}{dt} F = \frac{\partial}{\partial q^I} F + \{F, \tilde{H}\}_P + \{F, \phi_A\}_P \lambda^A \approx \frac{\partial}{\partial t} F + \{F, H\}_P, \]  

(A.7)

where the weak equality \(\approx\) in (A.7) holds once the constraints (A.5) are imposed, and Poisson brackets are defined as

\[ \{F, G\}_P \equiv \frac{\partial F}{\partial q^I} \frac{\partial G}{\partial p^J} - \frac{\partial F}{\partial p^J} \frac{\partial G}{\partial q^I}, \quad \forall \, F(q^I, p^J, t), \, G(q^I, p^J, t). \]  

(A.8)

The term with \(\phi_A\) in (A.7) appears due to the requirement that the variations must be taken on the constraint surface defined by (A.5). In order for the constraints (A.5) to hold throughout the time evolution (on the constraint surface), we require the following consistency conditions; substituting \(\phi_A\) into \(F\) in (A.7), we have

\[ \frac{d}{dt} \phi_A = \frac{\partial}{\partial t} \phi_A + \{\phi_A, \tilde{H}\}_P + \{\phi_A, \phi_B\}_P \lambda^B \approx 0. \]  

(A.9)

run through infinity, and \(\int dt L\) is replaced by \(\int d^4x L\), where \(L\) is a Lagrangian density. In principle, it is not guaranteed that the procedure described in this appendix ends by a finite number of steps for field theories, for which \(N\) is infinite.
While in some cases these conditions merely fix some Lagrange multipliers $\lambda^A$, in other cases they introduce additional constraints, called “secondary” constraints. To see this, we take the linear combinations of $\phi_A$ properly (such as done for $H^\text{tot}$ in the main text), to reduce the coefficient matrix $\{\phi_A, \phi_B\}_\text{P}$ in (A.9) to the form

$$
\{\phi_A, \phi_B\}_\text{P} = \left(\{\phi_\alpha, \phi_\beta\}_\text{P} \{\phi_a, \phi_b\}_\text{P}\right) \approx \begin{pmatrix} C_{\alpha\beta} & 0 \\ 0 & 0 \end{pmatrix},
$$

(A.10)

where $\det(C) \neq 0$, $A, B = 1, \ldots, M_1$, $\alpha, \beta = 1, \ldots, r_1$, $a, b = r_1 + 1, \ldots, M_1$, and $r_1 = \text{rank} (\{\phi_A, \phi_B\}_\text{P})$. Since any odd-dimensional antisymmetric matrix has vanishing determinant, $r_1$ here is always an even number. Since there exists the inverse matrix of $C_{\alpha\beta}$, $\lambda^a$ can be uniquely determined by

$$
\lambda^a = -(C^{-1})^{\alpha\beta} \left( \frac{\partial}{\partial t} \phi_\beta + \{\phi_\beta, \tilde{H}\}_\text{P} \right).
$$

(A.11)

On the other hand, we cannot determine the remaining $(M_1 - r_1)$ multipliers $\lambda^a$, as the conditions (A.9) for $\phi_a$ reduce to

$$
\frac{d}{dt} \phi_a = \frac{\partial}{\partial t} \phi_a + \{\phi_a, \tilde{H}\}_\text{P} \approx \frac{\partial}{\partial t} \phi_a + \{\phi_a, H\}_\text{P} \approx 0.
$$

(A.12)

If $d\phi_a/dt$ can be expressed as linear combinations of $\phi_A$, then no further procedure is necessary; otherwise, however, (A.12) will introduce the “secondary” constraints. If we obtain $M_2$ secondary constraints, we combine them with the primary constraints and extend the indices in (A.9) to $A, B = 1, \ldots, M_1 + M_2$. Then we repeat the steps (A.10)–(A.12) for the new set of constraints. Eq. (A.12) may again introduce further $M_3$ secondary constraints. Repeating this procedure until (A.12) produces no further constraint equations, we finally obtain $M = M_1 + M_2 + \cdots (\leq 2N)$ constraints and the coefficient matrix $\{\phi_A, \phi_B\}_\text{P}$ ($A, B = 1, \ldots, M$) whose rank is $r = r_1 + r_2 + \cdots (\leq M)$.

Adding the constraint terms, the “total” Hamiltonian is of the form

$$
H_\text{tot} = \tilde{H} + \phi_a \lambda^a + \phi_a \lambda^a,
$$

(A.13)

where $\lambda^a$ are determined by (A.11) (now $\alpha$ runs from 1 through $r$). The remaining $(M - r)$ multipliers $\lambda^a$ are yet to be determined. In order to fully determine them, we first define a useful terminology to distinguish $\phi^a$ from $\phi^\alpha$. We call any dynamical variable $R(q_I, p^J, t)$ first-class if $R$ satisfies

$$
\{R, \phi_A\}_\text{P} \approx 0, \quad A = 1, 2, \ldots, M,
$$

(A.14)

and otherwise we call it second-class. This definition is a slight extension of original Dirac’s one to the dynamical variables which can depend on time explicitly. According to this definition, the constraints $\phi^a$ are first-class, and $\phi^\alpha$ are second-class. As we have seen, the system contains the same number of undetermined coefficients $\lambda^a$ as that of the first-class constraints $\phi_a$. This in fact implies that $\phi_a$ are generators of gauge transformation of the system, under which all physical quantities must be invariant. The number of first-class constraints, $(M - r)$, is equal to the number of gauge symmetry, which in our case is spatial diffeomorphism. As gauge fixing, we can by hand impose additional $(M - r)$ constraints,

$$
\chi_a(q_I, p^J, t) \approx 0.
$$

(A.15)
We note that these gauge fixing conditions do not affect the second-class constraints since gauge symmetry does not change physics (or mathematically \( \{ \phi_a, \phi_\alpha \}_P \approx 0 \)). Then, we require the consistency conditions for \( \chi_a \) as in (A.9),

\[
\frac{d}{dt} \chi_a \approx \frac{\partial}{\partial t} \chi_a + \{ \chi_a, \tilde{H} + \phi_\alpha \chi^\alpha \}_P + \{ \chi_a, \phi_b \}_P \chi^b \approx 0 .
\] (A.16)

The choice of the gauge fixing conditions (A.15) should not be completely arbitrary, but rather they are to determine, through (A.16), the remaining Lagrange multipliers \( \lambda^a \), equivalently fixing the gauge completely. Therefore we require,

\[
\det |\{ \chi_a, \phi_b \}_P| \neq 0 ,
\] (A.17)

which leads to the relation,

\[
\det \begin{vmatrix} \{ \chi_a, \chi_c \}_P & \{ \chi_a, \phi_d \}_P \\ \{ \phi_b, \chi_c \}_P & \{ \phi_b, \phi_d \}_P \end{vmatrix} \approx \det^2 |\{ \chi_a, \phi_b \}_P| \neq 0 .
\] (A.18)

given \( \{ \phi_b, \phi_d \}_P \approx 0 \). Hence \( \phi_a \), together with \( \chi_a \), can now be treated as second-class constraints, and we can determine the remaining \( \lambda^a \) and the new Lagrange multipliers associated with the gauge-fixing constraints (A.15). We have therefore shown that once we fix the gauge completely and determine all the multipliers, we can solve for the motion of the system in that gauge, at least classically.

B Outline of calculating Poisson brackets

In the main text, we spared all the detailed calculations of the Poisson brackets and focused on the Hamiltonian structure of the theory. In this appendix, we outline some of the omitted part of the calculations. Among the Poisson brackets we have computed, the only non-trivial ones are \( \{ \bar{\mathcal{H}}, \bar{\mathcal{H}} \}_P \) and \( \{ \bar{\mathcal{H}}, \bar{\mathcal{C}} \}_P \) in (3.16) and (3.18), respectively (in principle, one may consider \( \{ \bar{\mathcal{C}}, \bar{\mathcal{C}} \}_P \), but there is no need to compute it in order to study the structure of the theory).

First it is useful to know the relation

\[
\sqrt{\hbar} D_i V^i = \partial_i \left( \sqrt{\hbar} V^i \right) ,
\] (B.1)

where \( V^i \) is an arbitrary vector. Thus if the expression on the left-hand side of (B.1) appears in the 3-integral \( \int d^3 x \), then it becomes total derivative. The relation (B.1) is used throughout the paper, whenever applicable.

The variations of \( \bar{\mathcal{H}} \) and \( \bar{\mathcal{C}} \) with respect to \( h_{ij} \) and \( \pi^{ij} \) are

\[
\frac{\delta \bar{\mathcal{H}}[f]}{\delta h_{ij}(z)} \approx \sqrt{\hbar} \left[ \frac{\pi^{ii}}{\sqrt{\hbar}} D_i f^j + \frac{\pi^{jl}}{\sqrt{\hbar}} D_j f^i - D_l \left( f^l \frac{\pi^{ij}}{\sqrt{\hbar}} \right) \right] ,
\] (B.2)

\[
\frac{\delta \bar{\mathcal{H}}[f]}{\delta \pi^{ij}(z)} \approx D_i f_j + D_j f_i ,
\] (B.3)
implies that the equality holds if \( \approx \). The term with the square brackets in (\( D \)) derivative. Hence we find the action by itself (up to constant coefficients).

From (\( \bar{\delta} \pi \)), it is immediate to see \( \sqrt{h} \) appears in (\( R \)) and \( \bar{\delta} R \delta \pi \), and the weak equality \( \approx \) implies that the equality holds if \( f^i \) and \( \varphi \) do not depend on \( h_{ij} \) or \( \pi^{ij} \). In order to derive (\( \ref{B.4} \)), we have used the variations of \( R_{ij} \) and \( R \), which are given by \( \delta R_{ij} = \frac{1}{2} h^{kl} (D_i \delta h_{jk} + D_j \delta h_{ik} - D_k \delta h_{ij}) - D_J D_i \delta \ln \sqrt{h} \), (\( \ref{B.6} \))

\[ \delta R = (R_{ij} + R_{ij} D^i - h^{ij} D^2) \delta h_{ij} \, . \tag{\( \ref{B.7} \)} \]

In principle \( \bar{\mathcal{C}} \) has non-vanishing variation with respect to \( N \) as well, but it is not needed for the current purpose, since \( \delta \frac{\bar{\mathcal{C}}}{\pi N} = 0 \).

Using (\( \ref{B.2} \)) and (\( \ref{B.3} \)), it is straightforward to show

\[ \{ \mathcal{H}[f], \mathcal{H}[g] \}_P \approx \int d^3x \left\{ 2 \sqrt{h} D_{ij} \left[ \epsilon^{ijk} \epsilon_{mnk} \left( f^m D_j g^n - g^m D_j f^n \right) \frac{\pi^{ij}_l}{\sqrt{h}} \right] \\ 
- 2 D_j \sqrt{h} \left( \frac{\pi^{ij}_l}{\sqrt{h}} \right) (f^j D_j g^l - g^j D_j f^l) \right\} . \tag{\( \ref{B.8} \)} \]

The term with the square brackets in (\( \ref{B.8} \)) has the structure of (\( \ref{B.1} \)) and thus is total derivative. Hence we find \( \{ \mathcal{H}[f], \mathcal{H}[g] \}_P \approx \mathcal{H} \left[ \left[ f, g \right] \right] \), as in (\( \ref{3.16} \)).

The calculation of \( \{ \mathcal{H}, \bar{\mathcal{C}} \}_P \) is more involved, yet straightforward. For the ease of the calculation, we remind of some properties of curvature tensors. The Bianchi identity with some indices contracted is often found useful; in particular,

\[ D_i R_{ij} - D_j R_{ij} = D_k R_{jli} \, , \tag{\( \ref{B.9} \)} \]

\[ D_j G^i_j = 0 \, . \tag{\( \ref{B.10} \)} \]

\footnote{From (\( \ref{B.7} \)), it is immediate to see \( \delta (\sqrt{h} R) = \sqrt{h} \left( -G^{ij} + D^j D^i - h^{ij} D^2 \right) \delta h_{ij} \), as expected. Note that the last two terms in the parentheses would be total derivatives if \( \sqrt{h} R \) appears in the action by itself (up to constant coefficients).}
The commutator of covariant derivatives introduces the curvature tensors; when acting on an arbitrary tensor, it is

$$[D_i, D_j] X^{m_1 \ldots m_a}_{n_1 \ldots n_b} = R^{m_1}_{k_1 j} X^{k m_2 \ldots m_a}_{n_1 \ldots n_b} + \ldots + R^{m_a}_{k_1 j} X^{m_1 \ldots m_{a-1} k}_{n_1 \ldots n_b} - R^{k}_{n_1 j} X^{m_1 \ldots m_a}_{k m_2 \ldots n_b} - \ldots - R^{k}_{n_1 j} X^{m_1 \ldots m_a}_{m k_2 \ldots n_1 n_{b-1} k} ,$$

(B.11)

since the connection in the present case is torsion free. Using these relations, one finds, up to total derivatives,

$$\{ \bar{\mathcal{H}}[f], \bar{\mathcal{C}}[\varphi] \}_P \approx \int d^3 x \sqrt{h} \left\{ \left( \frac{\pi^i \pi^j}{\hbar} - \frac{\pi^2}{2\hbar} \right) f^i D_i \varphi \frac{\partial}{\partial N} \left( \frac{N}{A_4} \right) + \frac{\pi}{2\hbar} f^i D_i \left[ \varphi \frac{\partial}{\partial N} \left( \frac{N A_3}{A_4} \right) \right] \right. \\
- \frac{3}{8} f^i D_i \left[ \varphi \frac{\partial}{\partial N} \left( \frac{N A_3^2}{A_4} \right) \right] + f^i D_i \left[ \varphi \frac{\partial}{\partial N} \left( N A_2 \right) \right] + R f^i D_i \left[ \varphi \frac{\partial}{\partial N} \left( N B_1 \right) \right] \\
- \frac{\pi \delta R_{ij} - \frac{1}{4} \pi R}{\hbar} f^i D_i \left[ \varphi \frac{\partial}{\partial N} \left( \frac{N B_3}{A_4} \right) \right] + R f^i D_i \left[ \varphi \frac{\partial}{\partial N} \left( \frac{N A_3 B_5}{8 A_4} \right) \right] \\
+ \left( R^m_n R^m_n - \frac{3}{8} R^2 \right) f^i D_i \left[ \varphi \frac{\partial}{\partial N} \left( \frac{N B_2^2}{4 A_4} \right) \right] \right\} .$$

(B.12)

We can rewrite this expression to be

$$\{ \bar{\mathcal{H}}[f], \bar{\mathcal{C}}[\varphi] \}_P \approx \int d^3 x \left( \mathcal{C} f^i D_i \varphi + \varphi f^i D_i N \frac{\partial}{\partial N} \mathcal{C} \right) .$$

(B.13)

The first term vanishes on the surface defined by $\mathcal{C} = 0$, but the second term does not. In order for $\mathcal{H}_i$ to be first-class constraints, therefore, we need to introduce another term in $\mathcal{H}_i$ to have

$$\mathcal{H}_i^{\text{tot}} \equiv \mathcal{H}_i + \pi_N \partial_i N ,$$

(B.14)

as in the main text. This new term cancels out the non-vanishing term in (B.13), giving

$$\{ \bar{\mathcal{H}}^{\text{tot}}[f], \bar{\mathcal{C}}[\varphi] \}_P \approx \bar{\mathcal{C}}[f \partial \varphi] ,$$

(B.15)

which concludes the proof of the calculations of the Poisson brackets in analyzing the Hamiltonian structure of the theory.

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