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Hamiltonian analysis of higher derivative scalar-tensor theories

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We perform a Hamiltonian analysis of a large class of scalar-tensor Lagrangians which depend quadratically on the second derivatives of a scalar field. By resorting to a convenient choice of dynamical variables, we show that the Hamiltonian can be written in a very simple form, where the Hamiltonian and the momentum constraints are easily identified. In the case of degenerate Lagrangians, which include the Horndeski and beyond Horndeski quartic Lagrangians, our analysis confirms that the dimension of the physical phase space is reduced by the primary and secondary constraints due to the degeneracy, thus leading to the elimination of the dangerous Ostrogradski ghost. We also present the Hamiltonian formulation for nondegenerate theories and find that they contain four degrees of freedom, as expected. We finally discuss the status of the unitary gauge from the Hamiltonian perspective.

I. INTRODUCTION

As a possible alternative explanation for the observed cosmological acceleration, theories of modified gravity have attracted considerable interest in the recent past (see e.g. [1–4] for reviews). Many, although not all, models of modified gravity are based on scalar-tensor theories, where one scalar degree of freedom is combined with the gravitational metric. The models that have been studied in the literature have progressively increased in complexity and generality, from quintessence models up to Lagrangians involving second-order derivatives of the scalar field. In the latter case, special care must be taken to avoid the so-called Ostrogradski instability [5]. Indeed, second or higher order time derivatives in the Lagrangian generically lead to the presence of an extra degree of freedom, which behaves like a ghost. It has long been believed that, in order to avoid Ostrogradski's ghost, it was necessary that the Lagrangian yields second-order equations of motion. This property is indeed satisfied for flat spacetime galileon [6]. When gravity is included, the same requirement led to the so-called generalized galileons [7, 8], which coincide with Horndeski theories [9, 10] in four dimensions.

The statement that second-order equations of motion are necessary to avoid ghost-like instabilities was first questioned in [11] by considering a theory obtained from Einstein-Hilbert via disformal transformation, and in [12], in the context of Horndeski theories, by proposing two extensions, denoted $L_4^{\rm bH}$ and $L_5^{\rm bH}$, of the quartic and quintic Horndeski Lagrangians $L_4^{\rm H}$ and $L_5^{\rm H}$ (further extensions, leading to Lorentz-breaking theories, were also proposed in [13]). It was later demonstrated in [14] that combinations of $L_4^{\rm H}$ and $L_4^{\rm bH}$, on one hand, or combinations of L_5^{H} and L_5^{bH}, on the other hand, can be related to a purely Horndeski Lagrangian via a disformal transformation, thus indicating that the number of degrees of freedom in these subclasses beyond Horndeski should be the same as in Horndeski theories. This brought further confirmation that at least some combinations of terms beyond Horndeski with Horndeski's ones were indeed healthy, although the status of arbitrary combinations of all terms remained uncertain.

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Further support was apparently provided by a recent work [15] in which it was shown that the third-order covariant equations of motion for the scalar field and the metric can be rewritten, in an arbitrary gauge, as a system of equations which are second-order in time derivatives. However, it is not fully clear what this implies about the number of degrees of freedom, as noted by the authors themselves. The same paper also presented a Hamiltonian treatment, in an arbitrary gauge, of the particular Lagrangian $L_4^{\rm bH}$ and showed that the number of degrees of freedom is strictly less than four.

In a previous paper [16], we reconsidered the question of the Ostrogradski ghost in higher derivative scalar-tensor theories from a different perspective, by focusing on the degeneracy of the Lagrangian. As we showed, the notion of degeneracy is much richer when a variable with second-order time derivatives is coupled to other degrees of freedom than when it is isolated. Working in an arbitrary coordinate system, we explored the degeneracy of a large class of scalar-tensor theories for which the Lagrangian depends quadratically on second derivatives of the scalar field. This class includes $L_4^{\rm H}$ and $L_4^{\rm bH}$ and we could thus demonstrate that these two Lagrangians are degenerate, as well as their sum. We also found other degenerate Lagrangians, which do not belong to the extensions beyond Horndeski introduced in [12].

Furthermore, we investigated the special case of $L_5^{\rm bH}$, which is cubic in second derivatives of the scalar field, and found that it is also degenerate, as well as the combination $L_4^{\rm bH}+L_5^{\rm bH}$. By contrast, we noticed that the combination $L_4^{\rm H}+L_4^{\rm bH}+L_5^{\rm bH}$ is *not* degenerate, which suggests that combinations of Horndeski terms with both quartic and quintic terms beyond Horndeski are not viable in general. Note that this result is compatible with the conclusions of [14] concerning disformal transformations since the above combination *cannot* be related to Horndeski via disformal transformation. However, it may seem at odds with the unitary gauge Hamiltonian analysis of [12, 14, 17], or rather its extrapolation for the quintic terms (as the detailed analysis was in fact restricted to the quartic terms). This apparent paradox is resolved by the fact that some nondegenerate, and thus unhealthy, theories can appear degenerate in the unitary gauge, as discussed in [16]. As the unitary gauge can sometimes be misleading, it is worth revisiting the Hamiltonian analysis of higher derivative theories by considering an arbitrary gauge and check whether we can confirm our conjecture that healthy theories, i.e. without Ostrogradski ghost, correspond to degenerate theories.

In this work, we present the full Hamiltonian analysis for the class of models studied in our previous work. By using appropriate dynamical variables, we are able to write the full Lagrangian in a relatively compact form, which greatly simplifies the computation of the Hamiltonian. The structure of the Hamiltonian is rather simple and exhibits, like in general relativity, a term linear in the lapse function and another linear in the shift. One thus recognizes the structure associated with spacetime diffeomorphisms invariance. This enables us to identify the first-class constraints generating the diffeomorphism invariance. For the detailed Hamiltonian analysis, one needs to distinguish between degenerate theories and nondegenerate ones. In the former case, the computation is a bit more involved because of the presence of a primary constraint between momenta, which in turn generates a secondary constraint. These two constraints, which are second-class, eliminate one degree of freedom in comparison with nondegenerate theories. One thus ends up with three degrees of freedom for degenerate theories, compared with the four degrees of freedom for nondegenerate theories.

This paper is organized as followed. In section 2, we present our general action and compute the full ADM decomposition of the action in an arbitrary gauge. In section 3, we focus on the kinetic terms of the Lagrangian, which we rewrite as a bilinear form acting on a 7-dimensional vector space. Section 4, which is the main section of this paper, is devoted to the Hamiltonian formulation of degenerate theories, the identification of first-class and second-class constraints and the counting of the number of degrees of freedom. In section 5, we repeat the same analysis for nondegenerate theories. We then discuss the unitary gauge in Section 6. We summarize our results

in the final section. Some technical details are given in three Appendices.

II. GENERAL ACTION AND $3+1$ ADM DECOMPOSITION

In this section, we perform the (3+1)-decomposition of the action, which is a prerequisite for the Hamiltonian analysis. We consider scalar-tensor actions of the form

$$S[g_{\mu\nu},\phi] \equiv \int d^4x\,\sqrt{|g|}\,[f\,\mathcal{R} + C^{\mu\nu\rho\sigma}\,(\nabla_\mu\nabla_\nu\phi)\,(\nabla_\rho\nabla_\sigma\phi)] \tag{2.1}$$

where $\mathcal{R}$ is the 4-dimensional Ricci scalar, and the tensor $C^{\mu\nu\rho\sigma}$, which depends only on ϕ and $\phi_\mu \equiv \nabla_\mu\phi$, can always be written as

$$\begin{aligned} C^{\mu\nu\rho\sigma} \;&\equiv\; \frac{1}{2}\alpha_1\,(g^{\mu\rho}g^{\nu\sigma} + g^{\mu\sigma}g^{\nu\rho}) + \alpha_2\,g^{\mu\nu}g^{\rho\sigma} + \frac{1}{2}\alpha_3\,(\phi^\mu\phi^\nu g^{\rho\sigma} + \phi^\rho\phi^\sigma g^{\mu\nu}) \\ &+\; \frac{1}{4}\alpha_4(\phi^\mu\phi^\rho g^{\nu\sigma} + \phi^\nu\phi^\rho g^{\mu\sigma} + \phi^\mu\phi^\sigma g^{\nu\rho} + \phi^\nu\phi^\sigma g^{\mu\rho}) + \alpha_5\,\phi^\mu\phi^\nu\phi^\rho\phi^\sigma . \end{aligned} \tag{2.2}$$

Here f and α_i are functions of ϕ and $X = \phi_\mu\phi^\mu$ only.

A. Particular cases

The class of theories (2.1) includes as a particular case the quartic Horndeski term

$$L_4^{\rm H} = G_4(\phi,X)\,{}^{(4)}R - 2G_{4,X}(\phi,X)(\Box\phi^2 - \phi^{\mu\nu}\phi_{\mu\nu})\,. \tag{2.3}$$

The above Lagrangian is indeed of the form (2.1)-(2.2) with

$$f = G_4\,, \qquad \alpha_1 = -\alpha_2 = 2G_{4,X}\,, \qquad \alpha_3 = \alpha_4 = \alpha_5 = 0\,. \tag{2.4}$$

The action (2.1) also includes the extension beyond Horndeski introduced in [12], which can be written as

$$L_4^{bH} = F_4(\phi,X)\epsilon^{\mu\nu\rho}{}_\sigma\,\epsilon^{\mu'\nu'\rho'\sigma}\phi_\mu\phi_{\mu'}\phi_{\nu\nu'}\phi_{\rho\rho'}\,. \tag{2.5}$$

This corresponds to (2.1)-(2.2) with

$$\alpha_1 = -\alpha_2 = XF_4\,, \qquad \alpha_3 = -\alpha_4 = 2F_4\,, \qquad \alpha_5 = 0\,. \tag{2.6}$$

Various aspects of these theories beyond Horndeski have been investigated recently (see e.g [18–31]).

B. ADM decomposition and notations

In the ADM formalism, the metric $ds^2 = g_{\mu\nu}dx^\mu dx^\nu$ is parametrized as follows

$$ds^2 \;=\; -N^2dt^2 + \gamma_{ij}(dx^i + N^idt)(dx^j + N^jdt)\,, \tag{2.7}$$

where N is the lapse function and N^i the shift vector. In matricial form, the metric $g_{\mu\nu}$ and its inverse $g^{\mu\nu}$ are given by

$$g_{\mu\nu} = \begin{pmatrix} -N^2 + \gamma_{ij}N^iN^j & \gamma_{ij}N^j \\ \gamma_{ij}N^i & \gamma_{ij} \end{pmatrix} \quad\text{and}\quad g^{\mu\nu} = \frac{1}{N^2}\begin{pmatrix} -1 & N^j \\ N^i & N^2\gamma^{ij} - N^iN^j \end{pmatrix}\,. \tag{2.8}$$

We also need to introduce the second fundamental form which is given by

$$K_{ij} = \frac{1}{2N}\left(\dot{\gamma}_{ij} - D_i N_j - D_j N_i\right) , \tag{2.9}$$

where D_i denotes the spatial covariant derivative associated with the spatial metric γ_{ij}.

In order to make the ADM decomposition of the action, it is convenient to replace second order derivatives that appear in (2.1) by first order derivatives via the introduction of new dynamical variables. We thus consider the new action

$$S[g_{\mu\nu}, \phi; A_\mu, \lambda^\mu] \equiv \int d^4x \sqrt{|g|}\left(f\,\mathcal{R} + C^{\mu\nu\rho\sigma}\nabla_\mu A_\nu\,\nabla_\rho A_\sigma\right) + \lambda^\mu(\nabla_\mu\phi - A_\mu), \tag{2.10}$$

which contains the auxiliary field A_μ, as well as the vector field λ^μ enforcing the relation

$$A_\mu = \nabla_\mu \phi\,. \tag{2.11}$$

Note that for $\mu = 0$, the previous relation is an equation of motion whereas it is a constraint for $\mu = i$. It is easy to show that this action is indeed equivalent to the original one (2.1) when one writes the Euler-Lagrange equations. In this new formulation, the tensor $C^{\mu\nu\rho\sigma}$ depends A_μ (and no longer on ϕ_μ).

Furthermore, as a consequence of (2.11), A_μ satisfies the symmetry relation $\nabla_\mu A_\nu = \nabla_\nu A_\mu$. When distinguishing temporal and spatial indices, this property allows us to replace all the terms $\nabla_0 A_i$ by $\nabla_i A_0$ in the action without changing the equations of motion, as shown explicitly in Appendix A.

C. Einstein-Hilbert term

We first present the ADM decomposition of the Einstein-Hilbert Lagrangian multiplied by a function of ϕ and $X = g^{\mu\nu}A_\mu A_\nu$, corresponding to the action

$$S_{EH} = \int d^4x \sqrt{|g|}\, f\,\mathcal{R}\,. \tag{2.12}$$

As is well-known, the (3+1) decomposition of this action yields

$$S_{EH} = \int dt\, d^3x\, N\sqrt{\gamma}\, f\,\left(K_{ij}K^{ij} - K^2 + R - 2\nabla_\mu(a^\mu - Kn^\mu)\right) , \tag{2.13}$$

where $\gamma \equiv \det(\gamma_{ij})$, R is the 3-dimensional Ricci scalar, K_{ij} is the second fundamental form (2.9) and $K = K^i_i$ is its trace. The last term in the action (2.13) involves the acceleration a^μ and the normal n^μ (of the spatial hypersurface Σ) whose components are

$$a^\mu = n_\nu \nabla^\nu n^\mu\,, \qquad n^\mu = \frac{1}{N}(1, -N^i)\,. \tag{2.14}$$

When f is constant, the last term in the action is a total derivative, which can be discarded. This term however becomes relevant when f depends on the scalar field or its derivatives. To perform the (3+1)-decomposition of this term, it is convenient to introduce the new variable

$$A_* \equiv A_\mu n^\mu = \frac{1}{N}(A_0 - N^i A_i)\,, \tag{2.15}$$

which corresponds to the normal component of A_μ with respect to the spatial hypersurface Σ.

After a straightforward calculation, we find

$$S_{EH} = \int dt\, d^3x\, N\sqrt{\gamma}\, \left(\frac{2}{N}\mathcal{B}^{ij}_{\rm grav} K_{ij}(\dot{A}_* - \Xi) + \mathcal{K}^{ij,kl}_{\rm grav} K_{ij}K_{kl} + 2\mathcal{C}^{ij}_{\rm grav} K_{ij} - \mathcal{U}_{\rm grav} \right) \tag{2.16}$$

where we have introduced the function

$$\Xi \equiv A^k D_k N + N^k D_k A_* \,, \tag{2.17}$$

and where the coefficients entering in the Lagrangian are given by

$$\begin{aligned}
\mathcal{B}^{ij}_{\rm grav} &= 2 f_{,X} A_* \gamma^{ij} \,, && (2.18)\\
\mathcal{K}^{ij,kl}_{\rm grav} &= \frac{1}{2} f(\gamma^{ik}\gamma^{jl} + \gamma^{il}\gamma^{jk} - 2\gamma^{ij}\gamma^{kl}) + 2 f_{,X}(\gamma^{ij}A^k A^l + \gamma^{kl}A^i A^j) \,, && (2.19)\\
\mathcal{C}^{ij}_{grav} &\equiv -\gamma^{ij}(2 f_{,X} A^k (D_k A_*) + f_{,\phi} A_*) \,, && (2.20)\\
\mathcal{U}_{\rm grav} &= -R + 2 D_i (f_{,X} D^i X + f_{,\phi} A^i) \,. && (2.21)
\end{aligned}$$

We use the notations $f_{,\phi} \equiv \partial f/\partial\phi$ and $f_{,X} \equiv \partial f/\partial_X$ for partial derivatives. All spatial indices are raised or lowered by the spatial metric γ_{ij}. In particular, we define $A^i \equiv \gamma^{ij}A_j$, so that $X = -A_*^2 + A_i A^i$.

D. Scalar-tensor interaction term

We proceed in a similar way to decompose the "scalar-tensor" interaction part of the action

$$S_\phi \equiv \int d^4x\, \sqrt{|g|} C^{\mu\nu\rho\sigma} \nabla_\mu A_\nu\, \nabla_\rho A_\sigma \,. \tag{2.22}$$

In that case, we need to compute the components of the tensor

$$A_{\mu\nu} \equiv \nabla_\mu A_\nu \equiv \partial_\mu A_\nu - \Gamma^\rho_{\mu\nu}\, A_\rho \,. \tag{2.23}$$

Using the expressions of the Christoffel symbols $\Gamma^\rho_{\mu\nu}$ in term of ADM quantities, given in Appendix B, one can easily obtain the different components of the covariant derivative of A_μ

$$\begin{aligned}
A_{00} &= N\dot{A}_* - \left(A_* N^i N^j + 2N A^{(i} N^{j)}\right) K_{ij} + N N^k D_k A_* + N^i N^j D_i A_j \\
&\qquad - N A^k D_k N + N^k(\dot{A}_k - D_k A_0) \,, && (2.24)\\
A_{i0} &= -(A_* N^j + N A^j) K_{ij} + N D_i A_* + N^k D_i A_k \,, && (2.25)\\
A_{0i} &= (\dot{A}_i - D_i A_0) - (A_* N^j + N A^j) K_{ij} + N D_i A_* + N^k D_i A_k \,, && (2.26)\\
A_{ij} &= D_i A_j - A_* K_{ij} \,. && (2.27)
\end{aligned}$$

As discussed in Appendix A, the terms $(\dot{A}_k - D_k A_0)$ and $(\dot{A}_i - D_i A_0)$, which appear in (2.24) and (2.26), can be eliminated. In this way, all the time derivatives of A_i disappear from the action.

Using the results of previous subsections and after a long calculation, one finds that the ADM decomposition of S_ϕ reduces to the following form

$$S_\phi = \int N\sqrt{\gamma}\left[\frac{\mathcal{A}}{N^2}(\dot{A}_* - \Xi)^2 + \frac{2}{N}\mathcal{B}^{ij}_\phi(\dot{A}_* - \Xi) K_{ij} + \mathcal{K}^{ijkl}_\phi K_{ij}K_{kl} + 2\mathcal{C}^{ij}_\phi K_{ij} + 2\frac{\mathcal{C}^0}{N}(\dot{A}_* - \Xi) - \mathcal{U}_\phi \right] \tag{2.28}$$

We have not labelled $\mathcal{A}$ and $\mathcal{C}_0$ with the subscript ϕ because such terms do not show up in the Einstein-Hilbert part of the action. The coefficients of the quadratic terms in time derivatives have already been computed in [16], and are given by[1]

$$\mathcal{A} = \alpha_2 + \alpha_1 - (\alpha_3 + \alpha_4)A_*^2 + \alpha_5 A_*^4 \,, \tag{2.29}$$

$$\mathcal{B}_\phi^{ij} = \frac{A_*}{2}\left(2\alpha_2 - \alpha_3 A_*^2\right)\gamma^{ij} - \frac{A_*}{2}\left(\alpha_3 + 2\alpha_4 - 2\alpha_5 A_*^2\right) A^i A^j \,, \tag{2.30}$$

$$\begin{aligned}\mathcal{K}_\phi^{ij,kl} &= \alpha_1 A_*^2 \gamma^{i(k}\gamma^{l)j} + \alpha_2 A_*^2 \gamma^{ij}\gamma^{kl} - \frac{1}{2}\alpha_3 A_*^2\left(A^i A^j \gamma^{kl} + A^k A^l \gamma^{ij}\right) \\ &\quad -\alpha_1\left(A^i A^{(k}\gamma^{l)j} + A^j A^{(k}\gamma^{l)i}\right) + (\alpha_5 A_*^2 - \alpha_4) A^i A^j A^k A^l \,.\end{aligned} \tag{2.31}$$

The coefficients of the linear terms are

$$\begin{aligned}\mathcal{C}_\phi^{ij} &= A_*(D_k A_l)[-\alpha_1\gamma^{ik}\gamma^{jl} - \alpha_2\gamma^{kl}\gamma^{ij} + \frac{1}{2}\alpha_3(\gamma^{kl}A^iA^j - A^kA^l\gamma^{ij}) + \alpha_5 A^iA^jA^kA^l] \\ &\quad +(D_kA_*)[A^k((\alpha_4 - 2\alpha_5 A_*^2)A^iA^j + \alpha_3 A_*^2\gamma^{ij}) + \alpha_1(\gamma^{jk}A^i + \gamma^{ik}A^j)] \,, \\ \mathcal{C}^0 &= \frac{1}{2}(D_iA_j)[(2\alpha_5 A_*^2 - \alpha_3)A^iA^j + (\alpha_3 A_*^2 - 2\alpha_2)\gamma^{ij}] + (\alpha_3 + \alpha_4 - 2\alpha_5 A_*^2)A_*A^iD_iA_*\end{aligned} \tag{2.32}$$

Finally, the potential is given by

$$\begin{aligned}\mathcal{U}_\phi &= -(\alpha_1\gamma^{ik}\gamma^{jl} + \alpha_2\gamma^{ij}\gamma^{kl} + \alpha_3 A^iA^j\gamma^{kl} + \alpha_4 A^iA^k\gamma^{jl} + \alpha_5 A^iA^jA^kA^l)(D_iA_j)(D_kA_l) \\ &\quad -(4\alpha_5 A_*^2 - \alpha_4)A^iA^j(D_iA_*)(D_jA_*) - (\alpha_4 A_*^2 - 2\alpha_1)(D_iA_*)(D^iA_*) \\ &\quad +2A_*\left(2\alpha_5 A^iA^jA^kD_jA_k + \alpha_3 A^iD_jA^j + \alpha_4 A^jD_jA^i\right)D_iA_* \,.\end{aligned} \tag{2.33}$$

It is worth noticing that by using A_* instead of A_0, we have automatically absorbed time derivatives of the lapse and of the shift, which otherwise would appear explicitly in the action. In general, terms that depend on $\dot{N}$ or $\dot{N}^i$ indicate the presence of additional degrees of freedom, but this is not always the case, as illustrated explicitly, for disformal transformations, in [32] and discussed in more detail in [33].

E. Summary: full (3+1) decomposition of the action

Putting together all our previous results, we finally obtain the full (3+1) decomposition of the modified action (2.10):

$$\begin{aligned}S &= \int dt\, d^3x\, N\sqrt{\gamma}\left[\mathcal{A}\,V_*^2 + 2\mathcal{B}^{ij}V_*K_{ij} + \mathcal{K}^{ijkl}K_{ij}K_{kl} + 2\mathcal{C}^{ij}K_{ij} + 2\mathcal{C}^0V_* - \mathcal{U}\right] \\ &\quad + \int dt\, d^3x\,(p_\phi\dot{\phi} - Np_\phi A_* - N^ip_\phi A_i + \lambda^i(\phi_i - A_i))\end{aligned} \tag{2.34}$$

where we have introduced the quantity

$$V_* \equiv \frac{1}{N}(\dot{A}_* - \Xi) \,. \tag{2.35}$$

The coefficients are given by

$$\mathcal{B}^{ij} = \mathcal{B}^{ij}_{\rm grav} + \mathcal{B}^{ij}_\phi \;\;,\;\; \mathcal{K}^{ijkl} = \mathcal{K}^{ijkl}_{\rm grav} + \mathcal{K}^{ijkl}_\phi \;\;,\;\; \mathcal{C}^{ij} = \mathcal{C}^{ij}_{\rm grav} + \mathcal{C}^{ij}_\phi \;\;,\;\; \mathcal{U} = \mathcal{U}_{\rm grav} + \mathcal{U}_\phi \,. \tag{2.36}$$

[1] Our definitions for $\mathcal{A}$ and $\mathcal{B}^{ij}$ in [16] differ from the present ones by factors of the lapse N.

In particular, the tensorial structure of the coefficients $\mathcal{B}^{ij}$ and $\mathcal{K}^{ijkl}$, which appear in the kinetic part of the action, depends only on the metric γ_{ij} and the vector A_i:

$$\mathcal{B}^{ij} = \beta_1 \gamma^{ij} + \beta_2 A^i A^j \tag{2.37}$$

$$\begin{aligned}\mathcal{K}^{ij,kl} &= \kappa_1 \gamma^{i(k}\gamma^{l)j} + \kappa_2\, \gamma^{ij}\gamma^{kl} + \frac{1}{2}\kappa_3 \left(A^i A^j \gamma^{kl} + A^k A^l \gamma^{ij} \right) \\ &\quad + \frac{1}{2}\kappa_4 \left(A^i A^{(k}\gamma^{l)j} + A^j A^{(k}\gamma^{l)i} \right) + \kappa_5 A^i A^j A^k A^l \,,\end{aligned} \tag{2.38}$$

with

$$\beta_1 = \frac{A_*}{2}(2\alpha_2 - \alpha_3 A_*^2 + 4 f_{,X}) \,, \quad \beta_2 = \frac{A_*}{2}(2\alpha_5 A_*^2 - \alpha_3 - 2\alpha_4) \tag{2.39}$$

$$\kappa_1 = \alpha_1 A_*^2 + f \,,\, \kappa_2 = \alpha_2 A_*^2 - f \,,\, \kappa_3 = -\alpha_3 A_*^2 + 4 f_{,X} \,,\, \kappa_4 = -2\alpha_1 \,,\, \kappa_5 = \alpha_5 A_*^2 - \alpha_4 \,. \tag{2.40}$$

In anticipation of the Hamiltonian analysis, we have changed the notation λ^0 into p_ϕ. Note that the coefficients $\mathcal{A}$ and $\mathcal{C}^0$ are unaffected by the gravitational part of the action.

III. KINETIC TERMS AND DEGENERACY CONDITION

The kinetic part of the action is given by the expression

$$S_{\rm kin} = \int dt\, d^3x\, N \sqrt{\gamma}\, \mathcal{L}_{kin} \;\text{ with }\; \mathcal{L}_{\rm kin} = \mathcal{A}\, V_*^2 + 2\mathcal{B}^{ij} V_* K_{ij} + \mathcal{K}^{ij,kl} K_{ij} K_{kl} \,, \tag{3.1}$$

where $\mathcal{L}_{\rm kin}$ can be viewed as a bilinear form acting on a 7-dimensional vector space (the vector space of 3×3 symmetric matrices is 6-dimensional). For a better understanding of the structure of the kinetic terms, it is instructive to introduce a basis where $\mathcal{L}_{\rm kin}$ can be diagonalized, or at least block diagonalized.

A. Metric kinetic terms

Let us first concentrate on $\mathcal{K}^{ij,kl}$ which defines a bilinear form on the 6-dimensional space of (3×3) symmetric real matrices Sym(3), or, equivalently, a linear map

$$\mathcal{K} : \text{Sym}(3) \longrightarrow \text{Sym}(3) \quad , \quad U \longmapsto \mathcal{K}U \;\text{ s.t. }\; (\mathcal{K}U)^{ij} = \mathcal{K}^{ij,kl} U_{kl} \,. \tag{3.2}$$

The space Sym(3) is naturally endowed with the scalar product

$$\langle U, V \rangle = U_{ij} \gamma^{jk} V_{kl} \gamma^{li} = U_{ij} V^{ij} \,, \tag{3.3}$$

and one can try to construct an orthonormal basis of Sym(3), with respect to this scalar product, in which $\mathcal{K}$ takes a simple form. To do so, let us introduce two unit spatial vectors u^i and v^j so that they form, together with the normalized vector $A^i/\|A\|$ (where $\|A\| = \sqrt{A^2}$), a complete orthonormal basis in 3-dimensional space, i.e. such that

$$u^i u_i = v^i v_i = 1 \;\;,\;\; u^i v_i = v^i A_i = A^i u_i = 0 \,. \tag{3.4}$$

By using these vectors, one can build an orthonormal basis of Sym(3), which consists of the following independent 6 matrices U^I:

$$U^1_{ij} = \frac{1}{\|A\|^2} A_i A_j \quad , \quad U^2_{ij} = \frac{1}{\sqrt{2}}(\gamma_{ij} - U^1_{ij}) \quad , \quad U^3_{ij} = \frac{1}{\sqrt{2}}(u_i u_j - v_i v_j) \,,$$

$$U^4_{ij} = \frac{1}{\sqrt{2}}(u_i v_j + u_j v_i)\ , \quad U^5_{ij} = \frac{1}{\sqrt{2}\|A\|}(u_i A_j + u_j A_i)\ , \quad U^6_{ij} = \frac{1}{\sqrt{2}\|A\|}(v_i A_j + v_j A_i)\,. \tag{3.5}$$

An immediate calculation shows that $\mathcal{K}$ is block diagonal in this basis. Indeed the four vectors U^I for $I \in \{3,4,5,6\}$ are eigenvectors of $\mathcal{K}$, while the subspace spanned by (U^1, U^2) is stable under the action of $\mathcal{K}$. More precisely, we have

$$\mathcal{K}\, U^1 = aU^1 + cU^2 \ \ , \ \ \mathcal{K}\, U^2 = cU^1 + bU^2\,, \tag{3.6}$$

$$\mathcal{K}\, U^3 = \kappa_1 U^3\ ,\ \mathcal{K}U^4 = \kappa_1 U^4\ ,\ \mathcal{K}\, U^5 = (\kappa_1 + \frac{\|A\|^2}{2}\kappa_4)U^5\ ,\ \mathcal{K}\, U^6 = (\kappa_1 + \frac{\|A\|^2}{2}\kappa_4)U^6\,, \tag{3.7}$$

with

$$a = \kappa_2 + \kappa_1 + A^2(\kappa_3 + \kappa_4) + (A^2)^2\kappa_5\ ,\ \ b = \kappa_1 + 2\kappa_2\ \ ,\ \ c = \sqrt{2}(\kappa_2 + \frac{1}{2}\|A\|^2\kappa_3)\,. \tag{3.8}$$

We thus find that the 6×6 matrix associated with $\mathcal{K}$ is decomposed into a 2×2 matrix and a diagonal 4×4 matrix. Although it is immediate to diagonalize the 2×2 matrix corresponding to the subspace spanned by (U^1, U^2), it is not very useful as we now need to consider the seventh dimension associated with V_*.

B. Mixing with the scalar field

Interestingly, V_* mixes only with the projection of K_{ij} on the subspace (U^1, U^2), since the mixing coefficient $\mathcal{B}^{ij}$ is of the form

$$\mathcal{B} = (\beta_1 + A^2\beta_2)U^1 + \sqrt{2}\beta_1 U^2\,. \tag{3.9}$$

As a consequence, if we decompose K_{ij} according to

$$K_{ij} = K_I\, U^I_{ij}\ , \tag{3.10}$$

the kinetic term (3.1) can be written as

$$\mathcal{L}_{kin} \ = \ \mathcal{A}V_*^2 + V_*\left[(\beta_1 + A^2\beta_2)K_1 + \sqrt{2}\beta_1 K_2\right] + aK_1^2 + bK_2^2 + 2cK_1K_2 \tag{3.11}$$

$$+\kappa_1(K_3^2 + K_4^2) + (\kappa_1 + \frac{\|A\|^2}{2}\kappa_4)(K_5^2 + K_6^2)\,. \tag{3.12}$$

We thus find that the kinetic terms along the four directions U^I with $I \in \{3,4,5,6\}$, corresponding to the second line above, are trivial. The nontrivial part is embodied by the 3×3 matrix

$$\begin{pmatrix} \mathcal{A} & \frac{1}{2}(\beta_1 + A^2\beta_2) & \frac{1}{\sqrt{2}}\beta_1 \\ \frac{1}{2}(\beta_1 + A^2\beta_2) & a & c \\ \frac{1}{\sqrt{2}}\beta_1 & c & b \end{pmatrix}, \tag{3.13}$$

which mixes V_* with the metric velocities along γ_{ij} and A_iA_j.

C. Degeneracy

As discussed in detail in our previous paper [16], one encounters a degenerate theory when the kinetic part of the action corresponds to a degenerate quadratic form. In general, this degeneracy

could arise from the metric kinetic terms, i.e. from $\mathcal{K}$, if $\kappa_1 = 0$, $\kappa_1 = -\|A\|^2\kappa_4/2$ or $ab - c^2 = 0$. However, as we are mainly interested in theories which conserve two tensor modes, we focus our attention on theories where the degeneracy arises from the mixing with the scalar degree of freedom and we assume that $\mathcal{K}$ istself is nondegenerate.

In this case, $\mathcal{K}^{ij,kl}$ is invertible and the degeneracy condition reads [16]

$$\mathcal{A} - \mathcal{K}^{-1}_{ij,kl}\mathcal{B}^{ij}\,\mathcal{B}^{kl} = 0\,. \tag{3.14}$$

It is easy to check that this condition is equivalent to the requirement that the determinant of the 3×3 matrix (3.13) vanishes.

IV. HAMILTONIAN ANALYSIS FOR DEGENERATE THEORIES

A. Poisson bracket

We start the canonical analysis with the definition of the momenta associated to the dynamical variables, via the introduction of the Poisson brackets. With the (3+1) decomposition of the action, we see that the only non-trivial Poisson brackets for the gravitational degrees of freedom are

$$\{\gamma_{ij}, \pi^{kl}\} = \frac{1}{2}(\delta^k_i\delta^l_j + \delta^l_i\delta^k_j) \;\;,\;\; \{N, \pi_N\} = 1 \;\;,\;\; \{N^i, \pi_j\} = \delta^i_j\,, \tag{4.1}$$

and those for the scalar field degrees of freedom are

$$\{A_*, p_*\} = 1 \;\;,\;\; \{A_i, p^j\} = \delta^j_i \;\;,\;\; \{\phi, p_\phi\} = 1\,. \tag{4.2}$$

Note that we have identified the momentum conjugate to ϕ with $p_\phi = \lambda^0$. Furthermore, we have not introduced momenta for the variables λ^i which are clearly Lagrange multipliers, and thus are not dynamical variables. Even if the action does not contain any time derivative of A_i, N and N^i, we cannot a priori consider these variables as Lagrange multipliers, as they appear non linearly in the action. Nonetheless, we expect the lapse N and the shift N^i to be eventually Lagrange multipliers which impose symmetries under diffeomorphisms. As we will see, this is exactly what happens.

B. Primary constraints

As we have just emphasized, there is no time derivatives of the lapse and the shift in the action. This is due to the introduction of the variable A_* which automatically absorbs the time derivatives of these variables. Similarly, there is no time derivative of A_i and λ^i is a Lagrange multiplier. As a consequence, we get the following 10 primary constraints:

$$\pi_N \approx 0 \;\;,\;\; \pi_i \approx 0 \;\;,\;\; p^i \approx 0 \;\text{ and }\; \chi_i \equiv A_i - D_i\phi \approx 0\,, \tag{4.3}$$

where the symbol $\approx$ denotes weak equality (i.e. equality valid on the constraint surface). The momenta π^{ij} and p_*, respectively conjugate to γ_{ij} and A_*, can be expressed in terms of the configurational variables in the usual way,

$$p_* = 2\sqrt{\gamma}(\mathcal{A}V_* + \mathcal{B}^{ij}K_{ij} + \mathcal{C}^0)\,, \qquad \pi^{ij} = \sqrt{\gamma}(\mathcal{K}^{ij,kl}K_{kl} + \mathcal{B}^{ij}V_* + \mathcal{C}^{ij})\,. \tag{4.4}$$

The degeneracy condition (3.14) implies that p_* and π^{ij} are not independent and satisfy a primary constraint which can be written as

$$\Psi \;\equiv\; p_* - 2\mathcal{K}^{-1}_{ij,kl}\mathcal{B}^{kl}\pi^{ij} + 2\sqrt{\gamma}\left(\mathcal{K}^{-1}_{ij,kl}\mathcal{B}^{kl}\mathcal{C}^{ij} - 2\mathcal{C}^0\right) \approx 0\,. \tag{4.5}$$

At this point, we can conclude that, as $\mathcal{K}$ is invertible, there is no other primary constraint.

C. Total Hamiltonian

To go further in the analysis, we need to compute and simplify the expression of the total Hamiltonian $H_{\rm tot}$ defined by

$$\begin{aligned} H_{\rm tot} &= H + \int d^3x\,(\lambda^i\chi_i + \mu^N\pi_N + \mu^i\pi_i + m_i p^i + m\Psi) \quad \text{with} \\ H &\approx \int d^3x\,(p_*\dot{A}_* + \pi^{ij}\dot{\gamma}_{ij} + p_\phi\dot{\phi}) - L_0\,. \end{aligned} \tag{4.6}$$

Here μ^N, μ^i, m_i and m are Lagrange multipliers enforcing the primary constraints, $L_0 = L + \lambda^i\chi_i$ where L is the Lagrangian of the theory (we have suppressed the Lagrange multiplier part $\lambda^i\chi_i$ to rewrite it explicitly in the first line above). As a consequence,

$$\begin{aligned} H &= \int d^3x(p_*\dot{A}_* + \pi^{ij}\dot{\gamma}_{ij} - N\sqrt{\gamma}\mathcal{L}_0 + Np_\phi A_* + N^i p_\phi A_i) \quad \text{with} \\ \mathcal{L}_0 &= \mathcal{A}\,V_*^2 + 2\mathcal{B}^{ij}V_*K_{ij} + \mathcal{K}^{ijkl}K_{ij}K_{kl} + 2\mathcal{C}^{ij}K_{ij} + 2\mathcal{C}^0V_* - \mathcal{U}\,. \end{aligned} \tag{4.7}$$

To write the Hamiltonian in terms of the phase space variables, one needs to reexpress the velocities in terms of the momenta. To do so, we first note that, due to the degeneracy condition, the kinetic term in $\mathcal{L}_0$ factorizes according to

$$\mathcal{L}_0 = \mathcal{K}^{ij,kl}(K_{ij} + \mathcal{K}^{-1}_{kl,mn}\mathcal{B}^{mn}V_*)(K_{kl} + \mathcal{K}^{-1}_{kl,pq}\mathcal{B}^{pq}V_*) + 2\mathcal{C}^{ij}K_{ij} + 2\mathcal{C}^0\dot{A}_* - \mathcal{U}\,. \tag{4.8}$$

Inverting the second relation in (4.4) allows to express K_{ij} in terms of the momenta π^{ij} and $\dot{A}_*$,

$$K_{ij} = \mathcal{K}^{-1}_{ij,kl}(\frac{1}{\sqrt{\gamma}}\pi^{kl} - V_*\mathcal{B}^{kl} - \mathcal{C}^{kl})\,, \tag{4.9}$$

which can be substituted in the Lagrangian density $\mathcal{L}_0$. Furthermore, (4.9) allows to simplify the canonical terms of the Hamiltonian (4.7) as follows:

$$\begin{aligned} p_*\dot{A}_* + \pi^{ij}\dot{\gamma}_{ij} &= \frac{2N}{\sqrt{\gamma}}\mathcal{K}^{-1}_{ij,kl}\pi^{ij}\pi^{kl} - 2N\mathcal{K}^{-1}_{ij,kl}\pi^{ij}\mathcal{C}^{kl} + 2\pi^{ij}D_iN_j \\ &\quad + NV_*\left((p_* - 2\mathcal{K}^{-1}_{ij,kl}\pi^{ij}\mathcal{B}^{kl}\right) \end{aligned} \tag{4.10}$$

Putting everything together, we get the following expression for the Hamiltonian:

$$\begin{aligned} H &= \int d^3x\,N\sqrt{\gamma}\left[\mathcal{K}^{-1}_{ij,kl}\left(\frac{\pi^{ij}}{\sqrt{\gamma}} - \mathcal{C}^{ij}\right)\left(\frac{\pi^{kl}}{\sqrt{\gamma}} - \mathcal{C}^{kl}\right) + \mathcal{U}\right] + \\ &\quad + \int d^3x\left[\Xi\,p_* + Np_\phi A_* + N^i\left(p_\phi A_i - 2\sqrt{\gamma}D^j\left(\frac{\pi_{ij}}{\sqrt{\gamma}}\right)\right) + \sqrt{\gamma}V_*\Psi\right]\,. \end{aligned} \tag{4.11}$$

Note that the dependency on V_* disappears due to the primary constraint $\Psi \approx 0$. Furthermore, we show, after a direct calculation (and ignoring the surface terms that appear in the integration by parts), that the Hamiltonian takes the expected form

$$H \approx \int d^3x\,(N\mathcal{H}_0 + N^i\mathcal{H}_i)\,, \tag{4.12}$$

with

$$\mathcal{H}_0 = \sqrt{\gamma}\left[\mathcal{K}^{-1}_{ij,kl}\left(\frac{\pi^{ij}}{\sqrt{\gamma}} - \mathcal{C}^{ij}\right)\left(\frac{\pi^{kl}}{\sqrt{\gamma}} - \mathcal{C}^{kl}\right) + \mathcal{U} + \frac{p_\phi}{\sqrt{\gamma}}A_* - D_i\left(A^i\,\frac{p_*}{\sqrt{\gamma}}\right)\right]\,, \tag{4.13}$$

$$\mathcal{H}_i = -2\sqrt{\gamma}\,D^j\left(\frac{\pi_{ij}}{\sqrt{\gamma}}\right) + p_*D_iA_* + p_\phi D_i\phi\,. \tag{4.14}$$

Finally, the total Hamiltonian, which defines the time evolution, reads

$$H_{\rm tot} = \int d^3x \left(N\mathcal{H}_0 + N^i\mathcal{H}_i + \lambda^i\chi_i + \mu^N\pi_N + \mu^i\pi_i + m_i p^i + m\Psi \right) . \tag{4.15}$$

At this point, it is important to recall that one can replace any of the constraints by a new one which is a linear combination of the original ones, provided the new set of constraints remains complete (i.e. the linear transformation between the two sets of constraints is invertible). In particular, we can use this property to replace the variables A_i by $D_i\phi$ in each term of $H_{\rm tot}$, except χ_i. Furthermore, we use the constraint $\Psi \approx 0$ to replace everywhere, except in Ψ, the momentum p_* by its expression in terms of π^{ij}. To avoid heavy notations, we keep the same name for the modified constraints. In conclusion, the functions $\mathcal{H}_0$, $\mathcal{H}_i$ and Ψ now depend only on the gravitational degrees of freedom γ_{ij} and π^{ij}, on A_* and p_* as wellas on ϕ and p_ϕ, while the dependence on A_i has been eliminated.

D. Time evolution of the primary constraints and secondary constraints

We now study the time evolution of the primary constraints. Let us recall that the time evolution of any function F defined on the phase space is determined from the total Hamiltonian H_{tot}, according to

$$\dot{F} \equiv \{F, H_{tot}\} . \tag{4.16}$$

1. *Hamiltonian and momentum constraints*

Let us start with the primary constraints $\pi_N \approx 0$ and $\pi_i \approx 0$. One sees immediately that

$$\dot{\pi}_N \approx 0 \Longrightarrow \mathcal{H}_0 \approx 0 \quad \text{and} \quad \dot{\pi}_i \approx 0 \Longrightarrow \mathcal{H}_i \approx 0 , \tag{4.17}$$

and it is thus natural to expect that $\mathcal{H}_0 \approx 0$ and $\mathcal{H}_i \approx 0$ correspond to the usual Hamiltonian and momentum constraints of the theory and act as generators of the space-time diffeomorphisms.

It is easy to check that $\mathcal{H}_i$ generates the spatial diffeomorphisms. Its expression (4.14) is the usual one for a system involving gravity and several scalar fields. More precisely, if one considers the action of the smeared function

$$\mathcal{H}(\vec{N}) \equiv \int d^3x N^k \mathcal{H}_k , \tag{4.18}$$

on the variables A_*, ϕ and γ_{ij}, one easily gets

$$\{A_*, \mathcal{H}(\vec{N})\} = \mathcal{L}_{\vec{N}} A_* \ , \ \{\phi, \mathcal{H}(\vec{N})\} = \mathcal{L}_{\vec{N}}\phi \ , \ \{\gamma_{ij}, \mathcal{H}(\vec{N})\} = \mathcal{L}_{\vec{N}}\gamma_{ij} , \tag{4.19}$$

where $\mathcal{L}_{\vec{N}}$ is the Lie derivative in the direction $\vec{N} \equiv N^i\partial_i$.

The action of $\mathcal{H}(\vec{N})$ on the momenta is slightly different because conjugate momenta are densities of weight one. For example, p_* transforms as

$$\{p_*, \mathcal{H}(\vec{N})\} = \partial_i(N^i p_*) , \tag{4.20}$$

which is consistent with the fact that $p_*/\sqrt{\gamma}$ transforms as a scalar. Since $\mathcal{H}_0$ is also a scalar density, its transformation is similarly given by

$$\{\mathcal{H}_0, \mathcal{H}(\vec{N})\} = \partial_i(N^i\mathcal{H}_0) . \tag{4.21}$$

The Poisson brackets of the momentum constraints with themselves are given by

$$\{\mathcal{H}(\vec{N}_1), \mathcal{H}(\vec{N}_2)\} = \mathcal{H}(\vec{N})\,, \qquad N^i \equiv N_1^k D_k N_2^i - N_2^k D_k N_1^i\,. \tag{4.22}$$

The Poisson bracket of $\mathcal{H}_0$ with itself, or possibly of a redefined $\mathcal{H}_0$ combined with second-class constraints, is much more complicated to compute explicitly and we will simply assume, since our starting point is a Lagrangian invariant under four-dimensional diffeomorphisms, that it is given by the usual result

$$\{\mathcal{H}_0(N_1), \mathcal{H}_0(N_2)\} = \mathcal{H}(\vec{N})\,, \quad \text{with} \quad N^i \equiv N_1 D^k N_2 - N_2 D^k N_1\,, \tag{4.23}$$

where

$$\mathcal{H}_0(N) \equiv \int d^3x\, N\, \mathcal{H}_0 \tag{4.24}$$

is the smeared version of the Hamiltonian constraint. We have verified in a simple example that this is indeed the case (see Appendix C).

In conclusion, the time evolution of $\mathcal{H}_0 \approx 0$ and $\mathcal{H}_i \approx 0$ does not lead to new, i.e. tertiary, constraints.

2. *Fixing the Lagrange multipliers λ^i and m_i*

We now study the time evolution of the constraints $\chi_i \approx 0$ and $p^i \approx 0$. The essential ingredient here is the Poisson bracket

$$\{\chi_i, p^j\} = \delta_i^j\,, \tag{4.25}$$

which immediately implies that

$$\dot{\chi}_i = m_i - D_i(NA_* + N^j D_j \phi) \quad \text{and} \quad \dot{p}^i = -\lambda^i\,. \tag{4.26}$$

The time invariance of the constraints $\chi_i \approx 0$ and $p^i \approx 0$ thus fixes the Lagrange multipliers m_i and λ^i,

$$m_i = D_i(NA_* + N^j D_j \phi) \quad \text{and} \quad \lambda^i = 0\,, \tag{4.27}$$

and does not lead to secondary constraints.

It is interesting to notice that the Lagrange multiplier m_i can be rewritten, according to (2.15), as $m_i = D_i A_0 = D_i \dot{\phi} = \dot{A}_i$. When we replace this value in the action via the Hamiltonian (4.6), we obtain a new "canonical term"

$$m_i\, p^i = p^i \dot{A}_i\,, \tag{4.28}$$

which indicates that p^i and A_i are canonically conjugate variables. This is indeed how the p^i were defined initially, which confirms that the value that we get for the Lagrange multiplier m_i is fully consistent.

3. Secondary constraint from the time evolution of Ψ

It remains to consider the time evolution of the last primary constraint $\Psi \approx 0$. Because Ψ commutes with the other primary constraints χ_i, p^i, π_i and π_N, its evolution is simply given by

$$\dot{\Psi} = \{\Psi, \mathcal{H}_0(N)\} + \partial_i(N^i\Psi) \approx \{\Psi, \mathcal{H}_0(N)\}\,, \tag{4.29}$$

where we have used the property that Ψ is a scalar density and thus transforms like (4.20) under the action of $\mathcal{H}_i$. We thus obtain the secondary constraint

$$\Omega \equiv \{\mathcal{H}_0, \Psi\} \approx 0 \quad \text{with} \;\; \Omega = p_\phi + \Omega_{\text{rest}}. \tag{4.30}$$

The explicit form of Ω is rather involved in general but we do need its explicit form for our purpose. What matters is that it depends linearly on the variable p_ϕ as shown above, as Ω_{rest} does not contain p_ϕ. This means that the constraint Ω can be viewed as an equation that determines the momentum p_ϕ in terms of the other variables[2].

In order to complete the Dirac analysis, one must then compute the time evolution of Ω, which can be written in the form

$$\dot{\Omega} = \{\Omega, H_{\text{tot}}\} = \int d^3y\, m\, \{\Omega, \Psi\} + \{\Omega, H_{\text{tot}} - \int d^3y\, m\, \Psi\}\,, \tag{4.31}$$

where the second term in the last expression does not depend on m. In the generic case where $\Delta \equiv \{\Psi, \Omega\} \neq 0$, one thus finds that the Lagrange multiplier m is fixed by the time evolution of Ω, which does not generate any new constraint.

In the following, we will not consider the special situations where $\Delta \approx 0$, in which case one expects a tertiary constraint or a new symmetry of the theory. All this would amount to is a further reduction of the physical phase space. This means that the number of physical degrees of freedom that we are going to compute below, in the generic case, can be seen as an upper bound.

E. Number of physical degrees of freedom

Let us summarize our results. We started with a 30-dimensional phase space, spanned by ten pairs of conjugate variables describing the metric, given in (4.1), and five pairs of conjugate variables describing the scalar field, given in (4.2). By performing a Dirac analysis, we have identified 11 primary constraints (the 10 constraints in (4.3) and $\Psi \approx 0$, due to the degeneracy) and 5 secondary constraints ($\mathcal{H}_0 \approx 0$, $\mathcal{H}_i \simeq 0$ and $\Omega \approx 0$).

As in general relativity, the spacetime diffeomorphism invariance of the initial Lagrangian must translate into the presence of first-class constraints associated with time and space diffeormorphisms. We have showed that the $\mathcal{H}_i$ indeed generate spatial diffeomorphisms and argued that $\mathcal{H}_0$, possibly combined with second class constraints, should correspond to the Hamiltonian constraint that generates time reparametrisation. Furthermore, as none of the constraints depend on the lapse N and on the shift N^i, $\pi_N \approx 0$ and $\pi_i \approx 0$ are necessarily first-class constraints as well. We thus have 8 first-class constraints.

[2] It is not surprising that p_ϕ is a redundant variable, since the time derivative of ϕ is already contained in the variable A_*. The constraint Ω is the analog, from the Lagrangian point of view, of the definition of the momentum p_ϕ, i.e. $p_\phi = \partial\mathcal{L}/\partial\dot{\phi} = N^{-1}\partial\mathcal{L}/\partial A_*$. This relation may be rather complicated, in particular for $\mathcal{A} \neq 0$ where $\mathcal{L}$ depends on $\dot{A}_*$ quadratically, and on $\partial_i\dot{A}_*$ too. The explicit expression of p_ϕ in terms of phase space variables (or in terms of velocities) can thus be quite involved.

The remaining 8 constraints $\Phi_A = (p^i, \chi_i, \Psi, \Omega)$ form a family of second-class constraints, as we now show. We first recall that we have used of $\chi_i \approx 0$ to replace the variables A_i by $\partial_i\phi$ in all the constraints, except of course χ_i. With this in mind, it is immediate to see that the non-vanishing components of the Dirac matrix $M_{AB}(x,y) \equiv \{\Phi_A(x), \Phi_B(y)\}$ are given by

$$\{\chi_i(x), p^j(y)\} = \delta_i^j\, \delta(x-y)\ ,\ \{\Psi(x), \Omega(y)\} = \Delta\, \delta(x-y)\,,\ \{\chi_i(x), \Omega(y)\} = -\partial_{x^i}\delta(x-y)\,, \tag{4.32}$$

where we have made manifest the spatial dependence, due to the presence of the derivative of $\delta(x-y)$. Since $\Delta \neq 0$, the Dirac matrix is clearly invertible which means that Φ_A are second-class constraints. These constraints allow to eliminate the variables p^i and A_i and to reexpress p_* and p_ϕ in terms of γ_{ij}, π^{ij}, ϕ and A_* only. All other variables are redundant and can be eliminated by solving secondary constraints.

To conclude, let us compute the number of physical degrees of freedom. The dimension of the physical phase space is given by 30 - 2×(number of first class constraints) - (number of second class constraints)= $30 - 2\times 8 - 8 = 6$, which gives three degrees of freedom. As expected, this corresponds to two tensor modes and only one scalar degree of freedom. This confirms that the extra scalar degree of freedom associated with the Ostrogradski instability is not present in degenerate scalar-tensor theories.

V. NONDEGENERATE THEORIES

For completeness, let us turn to the case of nondegenerate theories. We reproduce the procedure followed in the previous section, starting with the action (2.34).

As before, our pairs of conjugate variables are defined by (4.1) and (4.2). The nondegeneracy of the Lagrangian, assumed in this section, implies that the relations between the momenta (p_*, π^{ij}) and the velocities, namely

$$\begin{pmatrix} \frac{p_*}{2\sqrt{\gamma}} - \mathcal{C}^0 \\ \frac{\pi^{ij}}{\sqrt{\gamma}} - \mathcal{C}^{ij} \end{pmatrix} = \begin{pmatrix} \mathcal{A} & \mathcal{B}^{kl} \\ \mathcal{B}^{ij} & \mathcal{K}^{ij,kl} \end{pmatrix} \begin{pmatrix} V_* \\ K_{kl} \end{pmatrix}\,, \tag{5.1}$$

can be inverted. This can be done explicitly by introducing the inverse of the kinetic matrix,

$$\begin{pmatrix} \mathcal{A} & \mathcal{B}^{kl} \\ \mathcal{B}^{ij} & \mathcal{K}^{ij,kl} \end{pmatrix}^{-1} \equiv \begin{pmatrix} \hat{\mathcal{A}} & \hat{\mathcal{B}}_{kl} \\ \hat{\mathcal{B}}_{ij} & \hat{\mathcal{K}}_{ij,kl} \end{pmatrix} \text{ with } \begin{cases} \hat{\mathcal{A}} = (\mathcal{A} - \mathcal{K}^{-1}_{ij,kl}\mathcal{B}^{ij}\mathcal{B}^{kl})^{-1} \\ \hat{\mathcal{B}}_{ij} = -\hat{\mathcal{A}}\,\mathcal{K}^{-1}_{ij,kl}\mathcal{B}^{kl} \\ \hat{\mathcal{K}}_{ij,kl} = \mathcal{K}^{-1}_{ij,kl} + \hat{\mathcal{A}}^{-1}\,\hat{\mathcal{B}}_{ij}\hat{\mathcal{B}}_{kl} \end{cases}. \tag{5.2}$$

Here there is no primary constraint between p_* and π_{ij} and the set of primary constraints reduces to (4.3). The total Hamiltonian of the theory is thus given by

$$\begin{aligned} H_{\rm tot} &= \int d^3x (p\dot{A}_* + \pi^{ij}\dot{\gamma}_{ij} - N\sqrt{|\gamma|}\mathcal{L}_0 + Np_\phi A_* + N^i p_\phi A_i) \\ &+ \int d^3x (\lambda^i\chi_i + \mu^N\pi_N + \mu^i\pi_i + m_i p^i)\,. \end{aligned} \tag{5.3}$$

A straightforward calculation easily leads to the following expression for the total Hamiltonian:

$$H_{\rm tot} = \int d^3x\, (N\mathcal{H}_0 + N^i\mathcal{H}_i + \lambda^i\chi_i + \mu^N\pi_N + \mu^i\pi_i + m_i p^i)\,, \tag{5.4}$$

where the Hamiltonian constraint $\mathcal{H}_0$ and the momentum constraints $\mathcal{H}_i$ are given by:

$$\mathcal{H}_0 = \frac{1}{\sqrt{\gamma}}(\frac{1}{4}\hat{\mathcal{A}}\,p_*^2 + \hat{\mathcal{B}}_{ij}p_*\pi^{ij} + \hat{\mathcal{K}}_{ij,kl}\pi^{ij}\pi^{kl}) +$$

$$+A_* p_\phi - \left(\hat{\mathcal{A}}\mathcal{C}^0 + \hat{\mathcal{B}}_{ij}\mathcal{C}^{ij}\right) p_* - 2\left(\mathcal{C}^0\hat{\mathcal{B}}_{kl} + \mathcal{C}^{ij}\hat{\mathcal{K}}_{ij,kl}\right)\pi^{kl} - \sqrt{\gamma}D_i\left(\frac{p_*}{\sqrt{\gamma}}D^i\phi\right)$$
$$+\sqrt{\gamma}\left[\mathcal{U} + 2\mathcal{C}^0\hat{\mathcal{B}}_{ij}\mathcal{C}^{ij} + \hat{\mathcal{K}}_{ij,kl}\mathcal{C}^{ij}\mathcal{C}^{kl}\right], \tag{5.5}$$

$$\mathcal{H}_i = -2\sqrt{\gamma}D^j\left(\frac{1}{\sqrt{\gamma}}\pi_{ij}\right) + p_* D_i A_* + p_\phi D_i\phi\,. \tag{5.6}$$

The analysis of the constraints is easier than in the degenerate case. Stability under time evolution of the constraints $\pi_N \approx 0$ and $\pi_i \approx 0$ leads to the secondary constraints which are the Hamiltonian and vectorial constraints. It is immediate to see that $\mathcal{H}_i$ is first-class and generates space diffeomorphims. As for $\mathcal{H}_0$, we show in Appendix C that it satisfies the expected Poisson algebra in a simple example. We expect this to be true in general and we thus assume that $\mathcal{H}_0$, combined with second-class constraints, is first-class. Stability under time evolution of $\chi_i \approx 0$ and $p_i \approx 0$ leads to fixing the Lagrange multipliers m_i and λ^i.

In summary, the theory admits 30 non-physical degrees of freedom (γ_{ij}, N, N^i, A_*, ϕ, A_i and their momenta) for 14 constraints. The constraints are divided into 8 first-class constraints ($\mathcal{H}_0$, $\mathcal{H}_i$, π_N and π_i) and 6 second-class constraints (p^i and χ_i). Thus, the theory admits 4 degrees of freedom (8 degrees of freedom in the phase space) which correspond to 2 tensorial degrees of freedom, 1 scalar and 1 ghost.

Exactly as in the degenerate case, we can solve explicitly the 6 second-class constraints by replacing everywhere in the theory A_i by ϕ_i and eliminating p^i. Furthermore, we can consider the lapse N and the shift N^i as Lagrange multipliers and thus eliminate the constraints $\pi_N \simeq 0$ and $\pi_i \simeq 0$. Finally, we end up with a theory that can be formulated in terms of 16 degrees of freedom in phase space (ϕ, A_*, γ_{ij} and their momenta) which satisfy 4 first-class constraints $\mathcal{H}_0 \approx 0$ and $\mathcal{H}_i \approx 0$.

VI. ON THE UNITARY GAUGE

In this section, we focus on the unitary gauge, which was used in the early Hamiltonian analyses of the theories beyond Horndeski [12, 14, 17], because of its simplicity. We will show that, in general, the unitary gauge is a good gauge, which breaks time reparametrization. However, there exist particular situations where the unitary gauge is not allowed because it leads to a singular Hamiltonian in the phase space region where the unitary gauge is imposed. These cases correspond to theories that are nondegenerate but look degenerate in the unitary gauge, such as those discussed in the Appendix of [16].

The unitary gauge consists in choosing the scalar field as the clock. More concretely, we impose a new primary constraint given by

$$\mathcal{F} \equiv \phi - t \approx 0\,. \tag{6.1}$$

We could have imposed ϕ to be an arbitrary monotonous function $f(t)$, but for simplicity we make the choice $f(t) = t$. Gauge fixing means that we consider a new theory with the total Hamiltonian

$$H_{\rm tot}^{\rm gauge} \equiv H_{\rm tot} + \int d^3x\, \xi\, \mathcal{F}\,, \tag{6.2}$$

where the Lagrange multiplier ξ enforces the gauge fixing (6.1). To see whether this is indeed an appropriate gauge fixing, we repeat the analysis of the constraints and verify that the symmetry under time reparametrization is indeed broken.

A. Unitary gauge in nondegenerate theories

Let us first consider nondegenerate theories with the Hamiltonian

$$H_{\rm tot} \;=\; \int d^3x \, (N\mathcal{H}_0 + N^i\mathcal{H}_i + \lambda^i\chi_i + \mu^N\pi_N + \mu_i\pi^i + m_i p^i) \, . \tag{6.3}$$

In the corresponding gauge fixed Hamiltonian (6.2), one can replace $\mathcal{H}_0$ and $\mathcal{H}_i$ by their respective expressions with $\partial_i\phi = 0$. Similarly, χ_i can be replaced by $\chi_i = A_i$. One thus finds that the expression of the total Hamiltonian simplifies drastically.

Stability under time evolution of χ_i and p^i fixes both Lagrange multipliers μ_i and λ^i, as in the arbitrary gauge case. To see the effect of the gauge fixing, it is sufficient to study the time evolution of $\mathcal{F}$. As $\mathcal{F}$ depends explicitly on time, its time derivative is now given by

$$\dot{\mathcal{F}} \equiv \frac{\partial \mathcal{F}}{\partial t} + \{\mathcal{F}, H_{\rm tot}^{\rm gauge}\} \approx NA_* - 1 \, , \tag{6.4}$$

which leads to the new secondary constraint

$$\mathcal{G} \equiv NA_* - 1 \approx 0 \, . \tag{6.5}$$

Requiring the time invariance of $\mathcal{G}$ fixes the Lagrange multiplier μ^N. An analysis of the time evolution of the other constraints shows that they do not produce additional constraints.

Let us now examine the nature (first or second class) of the constraints. As expected, $\mathcal{H}_i \approx 0$ and $\pi_i \approx 0$ remain first-class because the invariance under space diffeomorphims is not broken. By contrast, $\mathcal{H}_0 \approx 0$ and $\pi_N \approx 0$ are no longer first-class and together with $\mathcal{F} \approx 0$ and $\mathcal{G} \approx 0$, $\chi_i \approx 0$ and $p^i \approx 0$, they form a set of second-class constraints. Note that p^i and χ_i commute with the four others and therefore can be treated separately (in fact, they can be solved explicitly and thus be ignored in the following). The Dirac matrix $M_{AB} = \{\Phi_A, \Phi_B\}$ associated with the remaining four constraints (with $\Phi_1 \equiv \mathcal{H}_0$, $\Phi_2 \equiv \pi_N$, $\Phi_3 \equiv \mathcal{F}$, $\Phi_4 \equiv \mathcal{G}$) is given by

$$\begin{pmatrix} 0 & 0 & -1/N & \{\Phi_1, \Phi_4\} \\ 0 & 0 & 0 & -1/N \\ 1/N & 0 & 0 & 0 \\ -\{\Phi_1, \Phi_4\} & 1/N & 0 & 0 \end{pmatrix} \tag{6.6}$$

because

$$\{\mathcal{H}_0, \mathcal{F}\} \approx -\frac{1}{N} \quad , \quad \{\mathcal{H}_0, \mathcal{G}\} = N\{\mathcal{H}_0, A_*\} \quad , \quad \{\mathcal{G}, \pi_N\} \approx -\frac{1}{N} \, . \tag{6.7}$$

For any finite value of the Poisson bracket which simplifies in the unitary gauge to

$$\{\mathcal{H}_0, A_*\} \;\approx\; \frac{1}{\sqrt{\gamma}}(\frac{1}{2N}\hat{\mathcal{A}}p_* + \hat{\mathcal{B}}_{ij}\pi^{ij}) \tag{6.8}$$

the Dirac matrix $M_{\alpha\beta}$ is invertible.

In conclusion, the above analysis shows that the unitary gauge $\mathcal{F} \approx 0$ is, in general, a valid gauge. However, it supposes that the Hamiltonian $H_{\rm tot}$ itself is well defined in the unitary gauge. When the coefficient $\mathcal{A} - \mathcal{K}^{-1}_{ij,kl}\mathcal{B}^{ij}\mathcal{B}^{kl}$ vanishes in the unitary gauge, even if the theory is nondegenerate, then the coefficient $\hat{\mathcal{A}}$ is infinite and the Hamiltonian becomes singular in the unitary gauge. It means that the unitary gauge is problematic for theories that are nondegenerate but look degenerate when restricted to $\partial_i\phi = 0$.

B. Unitary gauge in degenerate theories

For degenerate theories, the analysis of the unitary gauge is similar but a bit subtler due to the presence of the extra primary constraint $\Psi \approx 0$ (which generates the secondary constraint $\Omega \approx 0$). For that reason, we will give more details than in the non-degenerate case.

The Hamiltonian that appears in (6.2) is

$$H_{\rm tot} \;=\; \int d^3x \left(N\mathcal{H}_0 + N^i\mathcal{H}_i + \lambda^i\chi_i + \mu^N\pi_N + \mu_i\pi^i + m_i p^i + m\Psi \right). \tag{6.9}$$

The constraints $\mathcal{H}_0$, $\mathcal{H}_i$ and Ψ, given in (4.13), (4.14) and (4.5) respectively, simplify into

$$\mathcal{H}_0 \;=\; \frac{1}{\kappa_1\sqrt{\gamma}}\left(\pi^{ij}\pi_{ij} - \frac{\kappa_2}{\kappa_1+3\kappa_2}\pi^2\right) + A_*\left(\frac{2f_{,\phi}}{\kappa_1+3\kappa_2}\pi + p_\phi\right) + \sqrt{\gamma}\left(\frac{3\omega^2}{\kappa_1+3\kappa_2} + \mathcal{U}\right) \tag{6.10}$$

$$\mathcal{H}_i \;=\; -2D^j\pi_{ij} + p_* D_i A_* \tag{6.11}$$

$$\Psi \;=\; p_* - \frac{2\beta_1}{\kappa_1+3\kappa_2}\left(\pi + 3\sqrt{\gamma} f_{,\phi} A_*\right), \tag{6.12}$$

where $\pi = \pi^{ij}\gamma_{ij}$ is the trace of the momentum and we have used

$$\mathcal{K}^{ij,kl} \;=\; \kappa_1\gamma^{i(k}\gamma^{l)j} + \kappa_2\gamma^{ij}\gamma^{kl} \;\text{ and }\; \mathcal{K}^{-1}_{ij,kl} = \frac{1}{\kappa_1}\gamma_{i(k}\gamma_{l)j} - \frac{\kappa_2}{\kappa_1(\kappa_1+3\kappa_2)}\gamma_{ij}\gamma_{kl} \tag{6.13}$$

$$\mathcal{U} \;=\; -R - 4D_i(f_{,X}A_*D^iA_*) - (\alpha_4 A_*^2 - 2\alpha_1)(D_iA_*)(D^iA_*) \tag{6.14}$$

$$\mathcal{B}^{ij} \;=\; \beta_1\gamma^{ij} \;\text{ and }\; \mathcal{C}^{ij} = -f_{,\phi}A_*\gamma^{ij}. \tag{6.15}$$

Let us note that the unitary gauge can be used only if $\mathcal{K}^{ij,kl}$ remains invertible in this gauge, which means that κ_1 and $\kappa_1 + 3\kappa_2$ must be non-zero. When $\mathcal{K}^{ij,kl}$ becomes degenerate in the unitary gauge, then the Hamiltonian is ill-defined and thus the gauge is not safe. This happens when

$$\alpha_1 X - f = 0 \quad\text{or}\quad (\alpha_1 + 3\alpha_2)X + 2f = 0, \tag{6.16}$$

where we have used that $A_*^2 = -X$ in the unitary gauge.

The analysis of secondary constraints is similar to the non-degenerate case with the difference that time evolution of Ψ leads to the secondary constraint $\Omega \approx 0$ as expected. We still have the vectorial constraints $\mathcal{H}_i \approx 0$ and $\pi^i \approx 0$ which form a set of first-class constraints. It remains to study the following 6 constraints, which we denote $\Phi_A \approx 0$:

$$\Phi_1 = \mathcal{H}_0\,,\;\; \Phi_2 = \pi_N\,,\;\; \Phi_3 = \mathcal{F}\,,\;\; \Phi_4 = \mathcal{G}\,,\;\; \Phi_5 = \Psi,\;\; \Phi_6 = \Omega\,. \tag{6.17}$$

They must be second-class to ensure that the unitary gauge is applicable. We thus need to compute the determinant of the full Dirac matrix $\{\Phi_A, \Phi_B\}$, which is weakly equal to

$$\begin{pmatrix} 0 & 0 & -1/N & 0 & 0 & \{\Phi_1,\Phi_6\} \\ 0 & 0 & 0 & -1/N & 0 & 0 \\ 1/N & 0 & 0 & 0 & 0 & 1 \\ 0 & 1/N & 0 & 0 & N & 0 \\ 0 & 0 & 0 & -N & 0 & -\Delta \\ \{\Phi_6,\Phi_1\} & 0 & -1 & 0 & \Delta & 0 \end{pmatrix}. \tag{6.18}$$

An immediate calculation shows that its determinant is Δ^2/N^4 which is nonzero when $\Delta \neq 0$ as we assumed at the begining. This confirms that the unitary gauge is an appropriate gauge, provided the Hamiltonian is well defined.

VII. CONCLUSIONS

In this work, we have presented a Hamiltonian formulation of higher order theories of the form (2.1), both in the degenerate and nondegenerate cases. The degenerate case is especially important as it includes the quadratic Horndeski Lagrangian $L_4^{\rm H}$, as well as its extension beyond Horndeski $L_4^{\rm bH}$.

By using the variables introduced in our previous work, we have been able to compute the total Hamiltonian for degenerate and nondegenerate theories. In both cases, our Hamiltonian is linear in the lapse N and the shift N^i and thus reproduces the familiar structure of the GR Hamiltonian, enabling us to identify the Hamiltonian and momentum first-class constraints associated with the invariance under spacetime diffeomorphisms. The only caveat in our derivation is that we did not compute explicitly the Poisson brackets of the Hamiltonian constraint with itself in order to check the full recovery of the familiar algebra. Or, more precisely, we checked it only for a simple (nondegenerate) theory, where the brute force calculation is already quite involved. However, it is natural to believe that this result should be true in general.

Our analysis confirms the conjecture of our previous paper that degenerate theories of the form (2.1) should contain only three dynamical degrees of freedom whereas the dynamics of their nondegenerate counterparts should include an extra scalar degree of freedom, which is expected to behave as an Ostrogradski ghost. To our knowledge, this is the first derivation of the Hamiltonian formulation for the quadratic Horndeski Lagrangian $L_4^{\rm H}$, confirming the absence of an Ostrogradski ghost. In the special case of the Lagrangian $L_4^{\rm bH}$, our Hamiltonian formulation appears rather simpler than the one presented in [15], based on a completely different choice of canonical variables. Furthermore, our analysis also applies to the new degenerate theories identified in our previous work.

In the future, it would be interesting to extend the present results to a larger class of theories, in particular theories which are cubic in second derivatives of the scalar field, such as the quintic Horndeski and beyond Horndeski Lagrangians. However, the difficulty to invert explicitly the relation between the momenta and velocities might be an obstacle in practice. It would also be instructive to clarify the relation between the number of degrees of freedom and the order of the equations of motion. As a first step, it would be easier to study this question in the context of particle mechanics [34].

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Appendix A: Elimination of the time derivatives $\dot{A}_i$ in the Lagrangian

As mentioned in the main text, one can use the property $\nabla_\mu A_\nu = \nabla_\nu A_\mu$, which directly follows from the relation $A_\mu = \nabla_\mu \phi$ to replace all the terms $\nabla_0 A_i$ by $\nabla_i A_0$ in the action. Indeed, whenever one encounters an expression of the form $B^i \nabla_0 A_i$ in the Lagrangian, where B^i is an arbitrary

combination of the variables, one can always write

$$\int d^4x\, B^i \nabla_0 A_i = \int d^4x\, B^i \left[\nabla_0(A_i - \phi_i) + \nabla_0 \nabla_i \phi\right] \tag{A1}$$

$$= \int d^4x\, B^i \left[\nabla_0(A_i - \phi_i) + \nabla_i(\phi_0 - A_0) + \nabla_i A_0\right] \tag{A2}$$

$$= \int d^4x\, \left[-(\nabla_0 B^i)(A_i - \phi_i) - (\nabla_i B^i)(\phi_0 - A_0) + B^i \nabla_i A_0\right] , \tag{A3}$$

where the last line is obtained via an integration by parts, leaving aside the boundary terms. Finally, after a redefinition of the variables λ^μ, one can check that the Lagrangian is unaffected by this change. We thus conclude that all the time derivatives of the spatial components A_i can be eliminated in the Lagrangian.

Appendix B: ADM decomposition of $\nabla_\mu A_\nu$

Here, we compute the components of the covariant derivative

$$\nabla_\mu A_\nu \equiv \partial_\mu A_\nu - \Gamma^\rho_{\mu\nu} A_\rho \tag{B1}$$

using the expressions of the Christoffel symbols $\Gamma^\rho_{\mu\nu}$ in term of ADM quantities. They are given by

$$\begin{aligned}
\Gamma^0_{00} &= \frac{1}{N}\left(N^i N^j K_{ij} + \dot{N} + N^i D_i N\right) , \\
\Gamma^k_{00} &= N N^i \left(2\gamma^{jk} - \frac{N^j N^k}{N^2}\right) K_{ij} + \dot{N}^k - \frac{N^k}{N}\dot{N} + N^i D_i N^k + N\left(\gamma^{kl} - \frac{N^k N^l}{N^2}\right) D_l N , \\
\Gamma^0_{0i} &= \frac{1}{N}\left(N^k K_{ki} + D_i N\right) , \\
\Gamma^j_{0i} &= N\left(\gamma^{jk} - \frac{N^j N^k}{N^2}\right) K_{ik} + D_i N^j - \frac{N^j}{N} D_i N , \\
\Gamma^0_{ij} &= \frac{1}{N} K_{ij} , \\
\Gamma^k_{ij} &= -\frac{N^k}{N} K_{ij} + \hat{\Gamma}^k_{ij} .
\end{aligned} \tag{B2}$$

In the last equation, $\hat{\Gamma}^k_{ij}$ denote the three-dimensional Christoffel symbols associated to the spatial metric γ_{ij}. From these expressions, one can easily obtain the different components of the covariant derivative of A_μ

$$\begin{aligned}
A_{00} &\equiv \nabla_0 A_0 = \dot{A}_0 - \Gamma^0_{00} A_0 - \Gamma^k_{00} A_k = N\dot{A}_* - \left(A_* N^i N^j + 2N A^{(i} N^{j)}\right) K_{ij} \\
&\quad + N N^k D_k A_* + N^i N^j D_i A_j - N A^k D_k N + N^k(\dot{A}_k - D_k A_0) , \qquad \text{(B3)} \\
A_{i0} &\equiv \nabla_i A_0 = D_i A_0 - \Gamma^0_{0i} A_0 - \Gamma^k_{0i} A_k = -(A_* N^j + N A^j) K_{ij} \\
&\quad + N D_i A_* + N^k D_i A_k , \qquad \text{(B4)} \\
A_{0i} &\equiv \nabla_0 A_i = \dot{A}_i - \Gamma^0_{0i} A_0 - \Gamma^k_{0i} A_k = (\dot{A}_i - D_i A_0) - (A_* N^j + N A^j) K_{ij} \\
&\quad + N D_i A_* + N^k D_i A_k , \qquad \text{(B5)} \\
A_{ij} &\equiv \nabla_i A_j = \partial_i A_j - \Gamma^0_{ij} A_0 - \Gamma^k_{ij} A_k = D_i A_j - A_* K_{ij} . \qquad \text{(B6)}
\end{aligned}$$

These expressions can also be directly obtained by projecting the 3+1 covariant decomposition of $\nabla_\mu A_\nu$, given in [16], onto a basis associated with the coordinates t and x^i.

Appendix C: Poisson bracket $\{\mathcal{H}_0, \mathcal{H}_0\}$

This goal of this Appendix is to verify that

$$\{\mathcal{H}_0(N_1), \mathcal{H}_0(N_2)\} = (N_1 D_i N_2 - N_2 D_i N_1)\mathcal{H}^i \,, \tag{C1}$$

for the special case

$$S[g_{\mu\nu}, \phi] \equiv \int d^4x \sqrt{|g|}\, (\mathcal{R} + \alpha(\nabla_\mu \nabla_\nu \phi)\, (\nabla^\mu \nabla^\nu \phi)) \;, \tag{C2}$$

where α is assumed to be constant. Note that this theory, which is of the form (2.2) with $f = 1$, $\alpha_1 = \alpha_2 = \alpha_3 = \alpha_4 = 0$ and $\alpha_5 = \alpha$, is nonegenerate.

According to (5.5), the smeared constraint $\mathcal{H}_0(N)$ is explicitly given by

$$\begin{aligned} \mathcal{H}_0(N) \;=\; & \int d^3x\, N \left[\frac{1}{\sqrt{\gamma}} (\frac{1}{4\alpha} p_*^2 + \mathcal{K}^{-1}_{ij,kl} \pi^{ij} \pi^{kl}) - 2\mathcal{C}^{ij} \mathcal{K}^{-1}_{ij,kl} \pi^{kl} + \sqrt{\gamma}(\mathcal{U} + \mathcal{K}^{-1}_{ij,kl} \mathcal{C}^{ij} \mathcal{C}^{kl}) + A_* p_\phi \right] \\ & + \int d^3x\, (D_i N) p_* \gamma^{ij} A_j \end{aligned} \tag{C3}$$

with

$$\mathcal{K}^{ij,kl} \;=\; (1 + \alpha A_*^2)\gamma^{i(k}\gamma^{l)j} - \gamma^{ij}\gamma^{kl} - \alpha(A^i A^{(k}\gamma^{l)j} + A^j A^{(k}\gamma^{l)j}) \,, \tag{C4}$$

$$\mathcal{C}^{ij} \;=\; -\alpha A_* D^i A^j + \alpha(A^i D^j A_* + A^j D^i A_*) \,, \tag{C5}$$

$$\mathcal{U} \;=\; -R - \alpha(D_i A_j)(D^i A^j) + 2\alpha(D_i A_*)(D^i A_*) \,. \tag{C6}$$

The Poisson bracket we wish to compute is given by

$$\begin{aligned} \{\mathcal{H}_0(N_1), \mathcal{H}_0(N_2)\} \;=\; & \int d^3x \left[\frac{\delta \mathcal{H}_0(N_1)}{\delta A_*} \frac{\delta \mathcal{H}_0(N_2)}{\delta p_*} + \frac{\delta \mathcal{H}_0(N_1)}{\delta \phi} \frac{\delta \mathcal{H}_0(N_2)}{\delta p_\phi} + \frac{\delta \mathcal{H}_0(N_1)}{\delta \gamma_{ij}} \frac{\delta \mathcal{H}_0(N_2)}{\delta \pi^{ij}} \right] \\ & - \; (N_1 \leftrightarrow N_2) \end{aligned} \tag{C7}$$

where $(N_1 \leftrightarrow N_2)$ means that one exchanges the role of N_1 and N_2 in the first line. For that purpose, we need to compute derivatives of $\mathcal{H}_0(N)$ with respect to the various phase space variables.

Derivatives with respect to the momenta are easy to compute:

$$\frac{\delta \mathcal{H}_0(N)}{\delta p_*} \;=\; N \frac{1}{2\alpha\sqrt{\gamma}} p_* + (D^i N) A_i \tag{C8}$$

$$\frac{\delta \mathcal{H}_0(N)}{\delta p_\phi} \;=\; N A_* \tag{C9}$$

$$\frac{\delta \mathcal{H}_0(N)}{\delta \pi^{ij}} \;=\; 2N \mathcal{K}^{-1}_{ij,kl} (\frac{\pi^{kl}}{\sqrt{\gamma}} - \mathcal{C}^{kl}) \tag{C10}$$

Derivatives with respect to the variables A_*, ϕ and γ_{ij} are more involved to compute, and it is useful to derive some intermediate results. Let us start with the derivatives with respect to A_i and A_* of the coefficients that appear in $\mathcal{H}_0(N)$. For $\mathcal{K}^{-1}_{ij,kl}$, we get

$$\frac{\partial \mathcal{K}^{ij,kl}}{\partial A_m} \;=\; -\alpha[\gamma^{im} A^{(k}\gamma^{l)j} + \gamma^{jm} A^{(k}\gamma^{l)i} + A^i \gamma^{m(k}\gamma^{l)j} + A^j \gamma^{m(k}\gamma^{l)i}] \tag{C11}$$

$$\frac{\partial \mathcal{K}^{-1}_{ij,kl}}{\partial A_*} \;=\; -2\alpha A_* \mathcal{K}^{-2}_{ij,kl} \tag{C12}$$

$$\frac{\partial \mathcal{K}^{-1}_{ij,kl}}{\partial A_m} \;=\; 2\alpha A^n \left[\mathcal{K}^{-1mp}_{ij} \mathcal{K}^{-1}_{np,kl} + \mathcal{K}^{-1mp}_{kl} \mathcal{K}^{-1}_{np,ij} \right] \tag{C13}$$

while the derivatives of $\mathcal{C}^{ij}$ are given by

$$\frac{\partial \mathcal{C}^{ij}}{\partial A_*} = -\alpha D^i A^j \,, \qquad \frac{\partial \mathcal{C}^{ij}}{\partial D_m A_*} = \alpha \left[A^i \gamma^{jm} + A^j \gamma^{im} \right] \tag{C14}$$

$$\frac{\partial \mathcal{C}^{ij}}{\partial A_m} = \alpha \left[\gamma^{mi} D^i A_* + \gamma^{mj} D^i A_* \right] \,, \qquad \frac{\partial \mathcal{C}^{ij}}{\partial D_m A_n} = -\alpha A_* \gamma^{i(k} \gamma^{l)j} \tag{C15}$$

and the derivatives of $\mathcal{U}$ by

$$\frac{\partial \mathcal{U}}{\partial D_m A_n} = -2\alpha D^m A^n \,, \qquad \frac{\partial \mathcal{U}}{\partial D_m A_*} = 4\alpha D^m A^n \,. \tag{C16}$$

Only terms which depend on derivatives of the metric will enter the Poisson bracket (C7). Indeed, $\mathcal{H}_0(N)$ does not depend on the derivatives of the momenta π^{ij} and (C7) is antisymmetric in the exchange $N_1 \leftrightarrow N_2$. Derivatives of the metric appear only in $\mathcal{U}$ through the 3 dimensional Ricci scalar R and $(D_i A_j)(D^i A^j)$, and also in $\mathcal{C}^{ij}$ through the covariant derivatives of A_i. Thus, we only need the following formulae:

$$\frac{\delta}{\delta \gamma_{ij}} \int d^3x N \sqrt{\gamma} R = N[\cdots]^{ij} + \sqrt{\gamma} \left[D^i D^j N - \gamma^{ij} D^m D_m N \right] \tag{C17}$$

$$\frac{\delta}{\delta \gamma_{ij}} \int d^3x N \sqrt{\gamma} (D_k A_l)^2 = N[\cdots]^{ij} + \sqrt{\gamma} (D_k N) [A^i (D^j A^k) + A^j (D^i A^k) - A^k D^i A^j] \tag{C18}$$

$$\frac{\delta}{\delta \gamma_{ij}} \int d^3x \, N \Theta_{kl} \, \mathcal{C}^{kl} = N[\cdots]^{ij} + \frac{\alpha}{2} A_* (D_k N) [A^k \Theta^{ij} - \Theta^{jk} A^i - \Theta^{ik} A^j] \tag{C19}$$

where Θ_{ij} is any tensor independent of derivatives of γ_{ij}. Terms proportional to N are not relevant for the calculation of (C7) and we do not need their explicit form.

Gathering the above results together, we obtain for $\delta \mathcal{H}_0(N)/\delta A_*$ the expression

$$\begin{aligned} \frac{\delta \mathcal{H}_0(N)}{\delta A_*} &= \frac{\partial \mathcal{H}_0(N)}{\partial A_*} - D_i \left[\frac{\partial \mathcal{H}_0(N)}{D_i \partial A_*} \right] \\ &= N p_\phi + 2\alpha N \sqrt{\gamma} \Big[-A_* \mathcal{K}^{-2}_{ij,kl} (\frac{\pi^{ij}}{\sqrt{\gamma}} - \mathcal{C}^{ij})(\frac{\pi^{kl}}{\sqrt{\gamma}} - \mathcal{C}^{kl}) \\ &+ \mathcal{K}^{-1}_{ij,kl} (D^i A^j)(\frac{\pi^{kl}}{\sqrt{\gamma}} - \mathcal{C}^{kl}) + 2 D_j [A_i \mathcal{K}^{-1ij}_{kl} (\frac{\pi^{kl}}{\sqrt{\gamma}} - \mathcal{C}^{kl})] - 2 D_i D^i A_* \Big] \\ &+ +4\alpha \sqrt{\gamma} (D_j N) \left[A_i \mathcal{K}^{-1ij}_{kl} (\frac{\pi^{kl}}{\sqrt{\gamma}} - \mathcal{C}^{kl}) - D^j A_* \right] . \end{aligned} \tag{C20}$$

For the two other derivatives, their component proportional to the lapse N does not contribute to the Poisson bracket (C7) because (C9) and (C10) are proportional to N. Thus, we concentrate only on the terms proportional to derivatives of the lapse and we obtain

$$\begin{aligned} \frac{\delta \mathcal{H}_0(N)}{\delta \phi} &= N[\cdots] - (D_i N) \sqrt{\gamma} D^i (\frac{p_*}{\sqrt{\gamma}}) - (D_i D^i N) p_* \\ &- 4\alpha \sqrt{\gamma} (D_m N) \left[\mathcal{K}^{-1ms}_{ij} \mathcal{K}^{-1}_{rs,kl} A^r (\frac{\pi^{ij}}{\sqrt{\gamma}} - \mathcal{C}^{ij})(\frac{\pi^{kl}}{\sqrt{\gamma}} - \mathcal{C}^{kl}) - \mathcal{K}^{-1mj}_{kl} (D_j A_*)(\frac{\pi^{kl}}{\sqrt{\gamma}} - \mathcal{C}^{kl}) \right] \\ &+ 2\alpha \sqrt{\gamma} [(D_m D_n N) - 2(D_m N) D_n] \left[A_* \mathcal{K}^{-1mn}_{kl} (\frac{\pi^{kl}}{\sqrt{\gamma}} - \mathcal{C}^{kl}) - D^n A^m \right] \end{aligned} \tag{C21}$$

and

$$\begin{aligned} \frac{\delta \mathcal{H}_0(N)}{\delta \gamma_{ij}} &= N[\cdots] - (D^i N) A^j p_* + \sqrt{\gamma} [(D^i D^j N) - \gamma^{ij} (D^k D_k N)] \\ &+ \alpha \sqrt{\gamma} (D_k N) \left[A_* (2 A^{(i} \mathcal{K}^{-1\,j)k}_{mn} - A^k \mathcal{K}^{-1\,ij}_{mn}) \frac{\pi^{mn}}{\sqrt{\gamma}} + \sqrt{\gamma} (A^k D^i A^j - 2 A^{(i} D^{j)} A^k) \right] . \end{aligned} \tag{C22}$$

We can now compute the various contributions to the Poisson bracket (C7). The part which is linear in p_ϕ is by far the easiest to compute. It has a contribution from (C20) only and is given by

$$\int d^3x[N_1(D^iN_2) - N_2(D^iN_1)]\, A_i\, p_\phi\,. \tag{C23}$$

The part linear in p_* receives contributions from the three components of the Poisson bracket (C7),

$$\begin{aligned}
\int d^3x \frac{\delta\mathcal{H}_0(N_1)}{\delta A_*}\frac{\delta\mathcal{H}_0(N_2)}{\delta p_*} &\to \int d^3x\, 2p_*[N_1(D^iN_2) - N_2(D^iN_1)]\left[D_iA_* - A^j\mathcal{K}^{-1}_{ij,kl}(\frac{\pi^{km}}{\sqrt{\gamma}} - \mathcal{C}^{kl})\right]\\
\int d^3x \frac{\delta\mathcal{H}_0(N_1)}{\delta \phi}\frac{\delta\mathcal{H}_0(N_2)}{\delta p_\phi} &\to \int d^3x\, [-N_1(D^iN_2) + N_2(D^iN_1)]\, p_*D_iA_*\\
\int d^3x \frac{\delta\mathcal{H}_0(N_1)}{\delta \gamma_{ij}}\frac{\delta\mathcal{H}_0(N_2)}{\delta \pi^{ij}} &\to \int d^3x\, 2p_*[N_1(D^iN_2) - N_2(D^iN_1)]A^j\mathcal{K}^{-1}_{ij,kl}(\frac{\pi^{kl}}{\sqrt{\gamma}} - \mathcal{C}^{kl})\,,
\end{aligned}$$

which give the total contribution

$$\int d^3x\, [N_1(D^iN_2) - N_2(D^iN_1)]\, p_*D_iA_*\,. \tag{C24}$$

The part linear in derivatives of π^{ij} has contributions from the three components of (C7) and is given by

$$[N_1(D_mN_2) - N_2(D_mN_1)]\sqrt{\gamma}\left[4\alpha A^mA_i\mathcal{K}^{-1in}_{kl} - A_*(1 + 2\alpha A_* + 2\gamma^{mn}\gamma^{ij})\mathcal{K}^{-1mn}_{kl}\right] D_n(\frac{\pi^{kl}}{\sqrt{\gamma}})$$

It is immediate the see that this expression reduces to

$$[N_1(D_mN_2) - N_2(D_mN_1)]\sqrt{\gamma}2\mathcal{K}^{mn,ij}\mathcal{K}^{-1}_{ij,kl}D_n(\frac{\pi^{kl}}{\sqrt{\gamma}}) \tag{C25}$$

which leads to

$$2[N_1(D_iN_2) - N_2(D_iN_1)]D_j(\frac{\pi^{ij}}{\sqrt{\gamma}})\,. \tag{C26}$$

Gathering (C23), (C24) and (C26) and checking that the other contributions (i.e. the terms quadratic in π^{ij}, those linear in π^{ij} and those independent of the momenta) vanish, we finally obtain

$$\{\mathcal{H}_0(N_1), \mathcal{H}_0(N_2)\} = [N_1(D_iN_2) - N_2(D_iN_1)]\mathcal{H}^i\,. \tag{C27}$$

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