The Cauchy problem and the initial data problem in effective theories of gravity

Áron D. Kovács

Supervisor: Prof. Harvey S. Reall

Department of Applied Mathematics and Theoretical Physics
University of Cambridge

This dissertation is submitted for the degree of
Doctor of Philosophy

Selwyn College

April 2021

Declaration

This dissertation is the result of my own work and includes nothing which is the outcome of work done in collaboration except as declared in the Preface and specified in the text. It is not substantially the same as any that I have submitted, or, is being concurrently submitted for a degree or diploma or other qualification at the University of Cambridge or any other University or similar institution except as declared in the Preface and specified in the text. I further state that no substantial part of my dissertation has already been submitted, or, is being concurrently submitted for any such degree, diploma or other qualification at the University of Cambridge or any other University or similar institution except as declared in the Preface and specified in the text.

As specified at the beginning of each chapter, the results presented in this thesis have been published in the following papers:

Á. D. Kovács, "Well-posedness of cubic Horndeski theories", Phys. Rev. D **100** (2019), no. 2 024005, [arXiv:1904.00963].

Á. D. Kovács and H. S. Reall, "Well-posed formulation of scalar-tensor effective field theory", Phys. Rev. Lett. **124** (2020) no. 22, 221101, [arXiv:2003.04327].

Á. D. Kovács and H. S. Reall, "Well-posed formulation of Lovelock and Horndeski theories", Phys. Rev. D **101** (2020), no. 12 124003, [arXiv:2003.08398].

Á. D. Kovács, "On the construction of asymptotically flat initial data in scalar-tensor effective field theory", [arXiv:2103.06895] (2021).

Áron D. Kovács
April 2021

The Cauchy problem and the initial data problem in effective theories of gravity

Áron D. Kovács

Abstract

Lovelock and Horndeski theories of gravity are diffeomorphism-invariant theories with second-order equations of motion. A subset of these theories can be motivated by effective field theory considerations and hence they could describe strong-field deviations from general relativity. In particular, the effects of some Horndeski theories might be observable by present and future gravitational wave detectors. To study the dynamics of the theories using numerical simulations, they must satisfy some mathematical consistency properties. In this thesis, we establish two such properties for Lovelock and Horndeski theories.

In the first part of the thesis, we study the Cauchy problem for Lovelock and Horndeski theories. To demonstrate that the Cauchy problem for a theory of gravity is locally well-posed, it is sufficient to show that the gauge-fixed equations of motion are strongly hyperbolic. First, we use some numerical-relativity-inspired gauge conditions to write the equations of motion of weakly coupled *cubic* Horndeski theories in a strongly hyperbolic form. Next, this result is strengthened by proving that any weakly coupled Lovelock and Horndeski theory possesses a strongly hyperbolic formulation. This is achieved by introducing a novel class of "modified harmonic" gauge conditions and gauge-fixing procedures.

Another essential requirement on a theory of gravity is the possibility to choose initial data that represents astrophysically realistic systems. Some of the physically most interesting systems are approximately isolated systems and can be modelled by asymptotically flat spacetimes. The second part of the thesis discusses three methods to construct such initial data for a class of Horndeski theories. These methods are based on standard conformal techniques used in general relativity to write the constraint equations as a system of elliptic partial differential equations. It is shown that for a class of weakly coupled Horndeski theories, the conformally formulated constraint equations admit a well-posed boundary value problem on asymptotically Euclidean initial data surfaces.

Acknowledgements

First and foremost, I would like to thank my supervisor, Harvey Reall, for giving me the opportunity to work on some very interesting problems under his guidance. His clear explanations and suggestions helped me become a better and more productive researcher. This thesis would not exist without his support, encouragement and patience.

I am also thankful to my friends at DAMTP for creating a stimulating environment that I have greatly benefited from. I enjoyed discussions with several people, including Fred Alford, Gabriele Benomio, Roland Bittleston, Philip Clarke, Mihalis Dafermos, Anne Davis, Felicity Eperon, Pau Figueras, Dejan Gajic, Owain Salter Fitz-Gibbon, István Kádár, Joe Keir, Hamed Masaood, Georgios Mavrogiannis, Filipe Miguel, Prahar Mitra, Giuseppe Papallo, Miren Radia, Justin Ripley, Jorge Santos, Paul Shellard, Wuhyun Sohn, Ulrich Sperhake, Rita Teixeira da Costa, Claude Warnick and Zoe Wyatt.

I would also like to thank some of my former teachers and professors who supported and inspired me to pursue theoretical physics, including Zoltán Csefkó, József Cserti, Gyula Dávid, Gábor Horváth, Sándor Katz, Géza Kiss, Lajos Pósa, Tibor Szokolai and Márta Táborné Vincze.

I am grateful to my loving parents for raising me in a supporting environment and making my education a priority; and to my brother for being the best friend I can imagine, despite the physical distance.

Finally, special thanks go to Eszter for bringing happiness into my life with her lovely presence.

Financial support

I acknowledge financial support from the George and Lilian Schiff Studentship.

Table of contents

Chapter 1

Introduction

Einstein's general relativity (GR) is regarded as one of the two pillars of modern physics, together with the Standard Model of particle physics. It provides an elegant geometrical description of gravity, it gives rise to a fascinating and rich phenomenology, and it is in excellent agreement with observations.

According to general relativity, spacetime is a 4-dimensional Lorentzian manifold M, with a metric tensor g and a Levi-Civita connection defined on it. The dynamics of spacetime is governed by Einstein's equation [1]

$$G_{ab} + \Lambda g_{ab} = 8\pi T_{ab} \tag{1.1}$$

where G_{ab} is the Einstein tensor and Λ is the cosmological constant. This equation relates the curvature of spacetime to the energy-momentum tensor T_{ab} of matter present in spacetime. As T_{ab} itself generally depends on the metric, the dynamics of matter and spacetime simultaneously influence each other (much like M. C. Escher's *Drawing Hands*).

In the limit of weak gravity and slowly moving matter, GR reduces to Newton's theory of gravity and is in accord with experimental tests performed in this regime (see e.g. [2] for a review).

The theory predicts that freely moving small test particles follow (timelike or null) geodesics of the curved spacetime (M, g). In particular, this means that the paths of light rays are "curved" lines in the vicinity of massive stars; this phenomenon is called light deflection. This result was experimentally confirmed by Eddington, and his colleagues in 1919 [3].

Another remarkable and robust prediction of GR is the existence and formation of black holes: regions of "no escape". Black holes can form by the gravitational collapse of matter (e.g. cold stars), as demonstrated by the singularity theorems of Penrose [4,5]. There are several landmark experimental results providing overwhelming evidence for the existence of black holes, including the monitoring of stellar orbitals around galactic centres [6, 7], the observation of the shadow of a black hole by the Event Horizon Telescope [8] or the direct detection of gravitational-wave signals emitted by coalescing binary black hole systems [9].

General relativity can also account for the large scale structure of the Universe, provided one includes dark energy (described by a small positive cosmological constant) and cold dark matter in the model.

Despite the long list of merits of GR, a few conceptual issues are awaiting resolution. As shown by Penrose and Hawking [4, 5, 10], the formation of curvature singularities inside black holes and in cosmological spacetimes is a generic feature of GR. The origin of the cosmological constant is unclear, and a satisfactory explanation for its "unnaturally" small value is still lacking. Moreover, GR is non-renormalizable as a quantum theory. These problems suggest that GR is only an effective theory valid up to some finite energy scale. To describe phenomena in the regime of extreme spacetime curvature, a more fundamental theory is needed that possibly unifies gravity with the other fundamental interactions and reproduces GR in the appropriate low energy limit. String theory is a candidate for such a theory, but a direct experimental probe of it (or other candidates) currently seems out of reach. Nevertheless, future observations (gravitational wave astronomy, in particular) may provide the first precision tests of GR in a strong field, highly dynamical regime.

1.1 Effective theories of gravity

To perform precision tests of GR using gravitational wave astronomy, we need theoretical templates for how a deviation from GR would affect the gravitational waves produced in a black hole (BH) merger. Producing such templates requires numerical relativity simulations of BH mergers in theories that modify GR in some way. But there are two problems with this. First: which theory should be simulated? Many theories of modified gravity have been proposed. Second: to perform numerical simulations, the theory must satisfy some mathematical consistency requirements.

Effective field theory (EFT) provides a possible solution to the first problem [11]. Without a preferred candidate for a UV-complete theory that modifies GR, we can parameterize our ignorance using the bottom-up EFT methodology of adding to the GR Lagrangian all possible higher derivative terms consistent with the desired field content and symmetries. Then one can use observations to constrain the coefficients of these terms. This provides a nice way of parameterizing small strong-field deviations from GR. The accuracy to which one has tested GR can be quantified by how small one has constrained the coefficients of the leading higher derivative terms to be.

In the effective action, operators containing higher derivatives are suppressed by powers of a strong coupling energy scale. To study low energy processes (i.e. at energies well below the strong coupling scale), it is sufficient to keep only the first few terms in the effective action. Therefore, the classical equations of motion of the weakly coupled, truncated effective theory are expected to describe low energy physics accurately. Although the corrections to the equations of motion arising from the higher derivative terms are small at weak coupling, these corrections may be important in certain situations. Small effects may accumulate over time, producing large observable deviations from the leading order theory [12].

As an example, consider first the EFT for vacuum gravity in d spacetime dimensions. In this EFT, the only dynamical field is the metric tensor, and the symmetries imposed on the theory are diffeomorphism-invariance and local Lorentz symmetry. The leading order term in the effective Lagrangian is the 2-derivative Einstein-Hilbert term

$$\mathcal{L}_{EH} = R. \tag{1.2}$$

There are three independent 4-derivative terms that can appear in the Lagrangian. The first two are R^2, $R^{\mu\nu}R_{\mu\nu}$. Since these involve the Ricci tensor, which appears in the equation of motion of the 2-derivative theory (Einstein's equation), these interactions are redundant and can be eliminated by field redefinitions [13]. The third 4-derivative term can be chosen to be the so-called Gauss-Bonnet invariant

$$\mathcal{L}_{GB} = \frac{1}{4}\delta^{\mu_1\mu_2\mu_3\mu_4}_{\nu_1\nu_2\nu_3\nu_4} R_{\mu_1\mu_2}{}^{\nu_1\nu_2} R_{\mu_3\mu_4}{}^{\nu_3\nu_4}. \tag{1.3}$$

where the generalized Kronecker delta is given by

$$\delta^{\rho_1\ldots\rho_q}_{\sigma_1\ldots\sigma_q} = q!\ \delta^{\rho_1}_{[\sigma_1}\delta^{\rho_2}_{\sigma_2}\ldots\delta^{\rho_q}_{\sigma_q]}. \tag{1.4}$$

If one truncates this EFT, retaining only the terms with up to 4 derivatives, the resulting theory is called Einstein-Gauss-Bonnet (EGB) theory. Thus, in the absence of matter, EGB theory gives the leading order EFT corrections to general relativity (GR) in $d > 4$ dimensions. Unfortunately, in $d = 4$ dimensions, the Gauss-Bonnet invariant is a total derivative, and hence it is a redundant term. Hence, in 4 dimensions, the leading higher derivative corrections to vacuum GR start at 6 derivatives [11].

The equation of motion of the resulting theory now involves higher than second derivatives of the metric. A generic feature of such (higher derivative) theories is that the Hamiltonian functional of the theories is unbounded. This result is referred to as Ostrogradsky-instability [14, 15]. It is often argued on physical grounds that theories suffering from the Ostrogradsky-instability admit unphysical ("runaway") solutions that are usually inconsistent with the regime of validity of the theory. Roughly speaking, the reason for this is that (in theories with Ostrogradsky-instability) even an initial configuration with small energy may evolve to a configuration in which large positive and negative energy modes are coupled. Hence, such theories may exhibit a significant energy cascade to the UV which is inconsistent with current observations.

Despite having pathological solutions, higher derivative theories may be valid in some restricted sense. There are standard ways of dealing with higher derivative equations when performing numerical simulations in simple EFTs, including the so-called reduction of order procedure [16] and the methods inspired by the Israel-Stewart approach to relativistic viscous hydrodynamics [17] (see also e.g. [18, 19] for a more recent summary of these ideas). It is worth emphasizing that rigorous mathematical results are still lacking on theories with higher derivative equations and on the validity of the approximations just mentioned, especially in the case of gravitational theories (see however e.g. [20] on relativistic viscous hydrodynamics and [21] for a more recent result on a scalar field model). Given the apparent difficulty of this problem, we shall restrict our attention in this thesis to gravitational EFTs with second-order equations of motion.

Now consider the case when we include matter coupled to gravity. The simplest case is GR minimally coupled to a scalar field. Following the EFT philosophy, one adds all possible higher derivative terms to the action. Assuming a parity symmetry, field redefinitions can be used to bring the action to the form [22]

$$S = \frac{1}{16\pi G}\int d^4x\sqrt{-g}\left(-V(\phi) + R + X + f_1(\phi)X^2 + f_2(\phi)\mathcal{L}_{\mathrm{GB}}\right) \tag{1.5}$$

where we have neglected terms with 6 or more derivatives, V, f_1, f_2 are arbitrary functions, $X = -(1/2)g^{\mu\nu}\partial_\mu\phi\partial_\nu\phi$ and $\mathcal{L}_{\rm GB}$ is given by (1.3). We will call this *4-derivative scalar-tensor theory* (4∂ST theory). The special case with $f_1(\phi) = 0$ is called Einstein-dilaton-Gauss-Bonnet (EdGB) theory.

The scalar-tensor theory (1.5) is also interesting from a physics point of view because its black hole solutions differ from the black hole solutions of vacuum GR for several choices of the coupling function $f_2(\phi)$ (see e.g. [23–29]). This may cause observable deviations from GR in a BH merger. EFT reasoning implies that the theory (1.5) is also relevant to cosmology e.g. in early Universe inflation [22].

If one imposes an additional symmetry that the equations of motion are invariant under shifts in ϕ then V and f_1 are constants and $f_2 = \lambda\phi$ where λ is a constant. The dimensionful constants f_1, λ then set a scale for UV physics.

Remarkably, the equations of motion of (1.5) are second order in derivatives: The theory has second-order equations of motion

$$
\begin{aligned}
E^\mu{}_\nu \quad \equiv \quad & G^\mu{}_\nu - \frac{1}{2}\left(X - V(\phi) + \epsilon_1 f_1(\phi)X^2\right)\delta^\mu_\nu - \frac{1}{2}(1 + 2\epsilon_1 f_1(\phi)X)\nabla^\mu\phi\nabla_\nu\phi \\
& + \left(\epsilon_2 f_2''(\phi)\nabla_{\nu_1}\phi\nabla^{\mu_1}\phi + \epsilon_2 f_2'(\phi)\nabla_{\nu_1}\nabla^{\mu_1}\phi\right)\delta^{\mu\mu_1\mu_2\mu_3}_{\nu\nu_1\nu_2\nu_3} R_{\mu_2\mu_3}{}^{\nu_2\nu_3} = 0 \qquad (1.6)
\end{aligned}
$$

$$
\begin{aligned}
E_\phi \quad \equiv \quad & -(1 + 6\epsilon_1 f_1(\phi)X)\Box_g\phi + V'(\phi) - 2\epsilon_1 f_1(\phi)\delta^{\mu_1\mu_2}_{\nu_1\nu_2}\nabla_{\mu_1}\phi\nabla^{\nu_1}\phi\nabla_{\mu_2}\nabla^{\nu_2}\phi \\
& + 3\epsilon_1 f_1'(\phi)X^2 - \frac{1}{4}\epsilon_2 f_2'(\phi)\delta^{\mu_1\mu_2\mu_3\mu_4}_{\nu_1\nu_2\nu_3\nu_4} R_{\mu_1\mu_2}{}^{\nu_1\nu_2} R_{\mu_3\mu_4}{}^{\nu_3\nu_4} = 0 \qquad (1.7)
\end{aligned}
$$

Hence it is free from "Ostrogradsky-ghosts". As mentioned above, neglect of terms in the action with 6 or more derivatives is justified only in the weakly coupled regime in which spacetime curvature and scalar field derivatives are small compared to the UV length scales introduced by coupling constants associated with the higher derivative corrections. Generically, this implies that the 4-derivative corrections to the equations of motion must also be small compared to the leading 2-derivative terms. It is only in this regime that we can trust EFT. Weak coupling is compatible with strong-field BH dynamics, as long as the size of the BHs is large compared to the UV length scales.

So far, we have only discussed the bottom-up EFT approach to build models that correct GR in a strong field regime. Another thing one might ask is whether the EGB or 4∂ST theories arise in a top-down approach from some candidate UV theory. It turns out that the Gauss-Bonnet coupling naturally shows up as a correction to the Einstein-Hilbert Lagrangian in a certain low energy limit of string theory [30, 31].

There are other examples of theory building in the literature that differ from the modern EFT approach. Given the pathologies associated with higher derivative equations of motion, it may seem natural to ask what is the most general theory with a given set of symmetries and fields that has second-order equations of motion.[1]

Lovelock theories of gravity are the most general theories in which the gravitational field is described by a single metric tensor satisfying a diffeomorphism invariant second-order equation of motion [32][2]. In vacuum, the equation of motion of a Lovelock theory in d spacetime dimensions is:

$$E^{\mu}{}_{\nu} \equiv G^{\mu}{}_{\nu} + \Lambda\delta^{\mu}_{\nu} + \sum_{p\geq 2} k_p \, \delta^{\mu\rho_1\ldots\rho_{2p}}_{\nu\sigma_1\ldots\sigma_{2p}} R_{\rho_1\rho_2}{}^{\sigma_1\sigma_2}\ldots R_{\rho_{2p-1}\rho_{2p}}{}^{\sigma_{2p-1}\sigma_{2p}} = 0 \tag{1.8}$$

where k_p are dimensionful coupling constants and we have scaled so that the coefficient of the Einstein term is unity[3]. For $d = 4$, the antisymmetrization implies that equation (1.8) reduces to the vacuum Einstein equation. For $d > 4$ Lovelock theories introduce finitely many new terms into the equation of motion. In particular, the term corresponding to $p = 2$ in (1.8) arises from the EGB Lagrangian (1.3).

Horndeski theories are the most general theories of a metric tensor coupled to a scalar field ϕ, with second order equations of motion, arising from a diffeomorphism-invariant action in $d = 4$ spacetime dimensions [35]. We will write the action of a Horndeski theory in the form

$$S = \frac{1}{16\pi G}\int \mathrm{d}^4x\sqrt{-g}\,(\mathcal{L}_1 + \mathcal{L}_2 + \mathcal{L}_3 + \mathcal{L}_4 + \mathcal{L}_5) \tag{1.9}$$

with

$$\begin{aligned}
\mathcal{L}_1 &= R + X - V(\phi)\\
\mathcal{L}_2 &= G_2(\phi, X)\\
\mathcal{L}_3 &= G_3(\phi, X)\Box\phi\\
\mathcal{L}_4 &= G_4(\phi, X)R + \partial_X G_4(\phi, X)\delta^{\mu\nu}_{\rho\sigma}\nabla_\mu\nabla^\rho\phi\nabla_\nu\nabla^\sigma\phi\\
\mathcal{L}_5 &= G_5(\phi, X)G_{\mu\nu}\nabla^\mu\nabla^\nu\phi - \frac{1}{6}\partial_X G_5(\phi, X)\delta^{\mu\nu\rho}_{\alpha\beta\gamma}\nabla_\mu\nabla^\alpha\phi\nabla_\nu\nabla^\beta\phi\nabla_\rho\nabla^\gamma\phi
\end{aligned}$$

[1] Of course, many of the possible interactions satisfying these criteria may be made redundant in EFT, using field redefinitions. It is also worth keeping in mind that our main reason to restrict to theories with second-order equations of motion in this thesis is the difficulty to tame equations with higher derivative operators.

[2] In some references, these theories are called Lánczos-Lovelock theories based on [33, 34].

[3] We will not consider Lovelock theories for which this coefficient vanishes.

where G_i $(i = 2, 3, 4, 5)$ are arbitrary coupling functions. Note that $\mathcal{L}_1$ is the action of Einstein gravity minimally coupled to a scalar field with potential V; we will refer to this as *Einstein-scalar field theory*. We could absorb the terms in $\mathcal{L}_1$ into other terms but we choose not to do so for later convenience. It can be shown that 4∂ST-theory is a Horndeski theory, although some work is required [36] to rewrite its action in the canonical form of a Horndeski theory.

So far, we have mainly focused on aspects of theory building and their physical motivations. However, to make predictions in an effective theory of gravity, the theory must satisfy some minimal mathematical requirements. We continue by addressing this issue and discussing a condition called the well-posedness of the initial value problem, which, apart from being important for mathematical consistency, is also necessary to solve the equations of motion of the theory numerically.

1.2 The initial value problem for hyperbolic PDEs

In this section, we review general results on the initial value problem (or Cauchy problem) of hyperbolic partial differential equations (PDEs). After a general discussion of the initial value problem based on [37–39], we define the different notions of hyperbolicity appearing in the literature. Then, we state some technical theorems on how hyperbolicity is related to the well-posedness of the Cauchy problem. Our treatment of first-order systems (sections 1.2.2-1.2.3) is based on [39–42]. The discussion of second-order systems (sections 1.2.4-1.2.5) is similar to the standard treatment appearing in e.g. [43]. The main reason for opting for a different presentation (which is based on Appendix A of the original research paper [44] done in collaboration with Harvey Reall) is to show that standard results on second-order systems can be obtained without using pseudodifferential calculus.

1.2.1 The initial value problem

Many classical physical theories are formulated in terms of a set of functions or fields whose behaviour is governed by a system of ordinary or partial differential equations. General solutions of the differential equations of classical physics often depend on free parameters or freely specifiable functions. This freedom is fixed by imposing suitable initial or boundary conditions, depending on the physical system of interest. In particular, it is natural to think about dynamical systems in terms of an initial value problem. Once an experimenter sets up appropriate initial conditions for a classical system, its subsequent evolution is expected to be deterministic, provided that it is left undisturbed.

For example, the motion of a set of non-relativistic point particles that interact with each other (and external forces) is governed by Newton's second law

$$\ddot{q}_I(t) = F_I\left(t, q_J(t), \dot{q}_J(t)\right) \tag{1.10}$$

where $\dot{q}$ stands for the derivative of q with respect to time, $\{q_I\}_{I=1}^N$ denote the coordinates of the particles, N is the number of degrees of freedom of the system and the functions $\{F_I\}_{I=1}^N$ denote the forces. Since the forces depend only on the coordinates and their first derivatives, this is a second-order system of ordinary differential equations (ODEs). Once the initial values of the coordinates and velocities

$$q_I(0) = q_I^{(0)}, \qquad\qquad \dot{q}_I(0) = v_I^{(0)} \tag{1.11}$$

are specified, (1.10) uniquely determines the motion of the particles at later times. More precisely, if the forces $F_I\left(t, q_J(t), \dot{q}_J(t)\right)$ are at least Lipschitz continuous in their second and third arguments then there exists a unique C^2 solution $q_I(t)$ at least for a short time (c.f. Cauchy-Lipschitz-Picard-Lindelöf theorem).

A simple example from classical field theory is the dynamics of a massless real scalar field $\phi(x)$ in 4-dimensional flat spacetime, obeying the massless Klein-Gordon wave equation

$$\Box\phi(x) \equiv \partial_\mu\partial^\mu\phi(x) = 0. \tag{1.12}$$

This is a second-order PDE, and thus we are free to set up initial data on the 3-dimensional hypersurface $x^0 = 0$ by specifying the initial spatial profile of the scalar field and its first time derivative:

$$\phi(0, x^i) = f(x^i), \qquad\qquad \partial_0\phi(0, x^i) = g(x^i). \tag{1.13}$$

The evolution of the scalar field is uniquely determined by equation (1.12) for $x^0 \geq 0$.

While it is expected from a viable classical theory to produce unique evolution from fixed initial data, it is is reasonable to demand more. For example, it is essential for predictivity that small perturbations in the initial conditions induce "small" deviations (in some sense) in the solution at later times. Another natural requirement (at least for relativistic theories) is to assert "causal propagation" of the field, in accord with relativity. To explain what this means, let us go back to the example of the massless scalar field. Assume that the initial data is changed outside a closed, compact subset S of the hypersurface $x^0 = 0$, but the data is left unaltered in S. Then the solution resulting from the new data agrees with the original one in the future domain of dependence of S, determined by the speed of light. This is because scalar wave solutions of (1.12) propagate with a finite speed (the speed of light).

Considering the above requirements, we say that an initial value problem is *well-posed* if (i) the system of differential equations describing the physical system of interest has a unique solution subject to suitable initial conditions, (ii) the solution depends continuously on the data and finally, (iii) variation of the initial data outside of a closed set leaves the solution unchanged in the future domain of dependence of S. A well-posed initial value formulation appears to be a reasonable mathematical consistency requirement to demand from a classical theory. However, as we explain in the remainder of this section, it comes with a few more subtleties.

Let us start by elaborating on condition (i) of the definition of well-posedness. Here, we need to be more precise about what qualifies as *suitable* initial data, or in other words, we need to decide what is an appropriate function space for adequate initial data. For example, if we accept analytic initial data, then we have the following theorem that would satisfy condition (i) of well-posedness.

Theorem 1.1 (Cauchy–Kovalevskaya theorem)**.** *Let $x^\mu = (x^0, x^i)$ be coordinates in $\mathbb{R}^d$ and consider the initial value problem for the following system of N first order partial differential equations*

$$\partial_0 U(x) = F(x, U, \partial U) \tag{1.14}$$

$$U(0, x^i) = f(x^i) \tag{1.15}$$

where U, F and f are N-component column vector valued functions. Suppose that f is analytic and F is an analytic function of its arguments. Then there exists a neighbourhood of the initial data surface $x^0 = 0$ so that there exists a unique analytic solution of the initial value problem (1.14)-(1.15)*. A similar statement holds for systems of PDEs of arbitrary order.*

The fundamental problem with restricting to analytic initial data, however, is that an analytic function is uniquely determined by its behaviour in the neighbourhood of a single point. Hence, it is not possible to vary analytic initial data outside a closed set S of the initial hypersurface without modifying the data in S. Thus the restriction to analytic initial data is not suitable to discuss causal propagation. Another shortcoming of the Cauchy-Kovalevskaya theorem is that it does not say anything about the dependence of the solution on the initial data, condition (ii) of well-posedness. Nevertheless, there are several other (less restrictive) function spaces that appear to be adequate. In this thesis, we will mainly focus on the case when the initial data is in a particular Sobolev space H^s.

Next, we expand on condition (ii). The choice of an appropriate function space allows us to make the notion of "small changes in the initial data" more precise. In the example of the massless scalar field, suppose that we have two solutions $\phi_1(x)$ and $\phi_2(x)$ arising from initial data

$$\phi_1(0,x^i) = f_1(x^i), \qquad \partial_0\phi_1(0,x^i) = g_1(x^i) \tag{1.16}$$

and

$$\phi_2(0,x^i) = f_2(x^i), \qquad \partial_0\phi_2(0,x^i) = g_2(x^i), \tag{1.17}$$

respectively, where $f_1, f_2 \in H^s$ and $g_1, g_2 \in H^{s-1}$. Then continuous dependence on the data could be expressed by an inequality of the form

$$||\phi_1 - \phi_2||_{H^s}(x^0) \leq C(x^0)||f_1 - f_2||_{H^s} + D(x^0)||g_1 - g_2||_{H^{s-1}} \tag{1.18}$$

where C and D are continuous functions.

As for condition (iii) of the definition of well-posedness, it is worth briefly commenting on a potential difficulty with the notion of domain of dependence. Some of the theories studied in the subsequent chapters exhibit a phenomenon called *multi-refringence*. This means that different degrees of freedom in the theory may have different speeds of propagation. Intuitively, it seems clear that the correct notion of domain of dependence appearing in condition (iii) above should be the one defined with respect to the "fastest" degree of freedom. However, the definition of domain of dependence is not so simple in the theories discussed in section 1.1. For more details, see section 3.5.2 and [45].

So far, we have referred to the simple linear wave equation (1.12) as an example. However, the issue of well-posedness is more subtle for nonlinear equations. A generic feature of these types of equations is that there may not exist global in time solutions for all data; solutions may blow up in a finite time. This can be illustrated with a simple example. Consider the problem

$$\partial_t\phi(t,x) = \phi(t,x)^2 \qquad\qquad \phi(0,x) = 1$$

where ϕ is a real scalar field. It is easy to write down the exact solution to this problem:

$$\phi(t,x) = (1-t)^{-1}$$

which blows up as $t \to 1$. Another simple example can be found in e.g. [46]. If the PDE has some special structure and one starts from a special type of initial data, then one may be able to do better. A famous example of this is the proof of nonlinear stability of Minkowski spacetime in GR, first proved by Christodoulou and Klainerman [47] (see [48] for a more recent and shorter proof). In their proof, they exploited the fact that the Einstein equations satisfy the so-called null condition and that the initial data is sufficiently close to that of flat space. Nevertheless, for generic initial data, the best one can hope for is to establish *local* well-posedness of nonlinear equations, which means proving existence, uniqueness and continuous dependence on the data for only a finite (but strictly non-zero) amount of time.

In the next few subsections, we will investigate the conditions under which the initial value problem of a system of PDEs is locally well-posed in the sense just discussed. Such equations are broadly referred to as *hyperbolic* equations.

1.2.2 Linear, constant coefficient equations

To illustrate the notion of hyperbolicity and its relation to the well-posedness of the initial value problem, it is worth exploring a simple setting: the case of a linear PDE with constant coefficients. Let $x^\mu = (x^0, x^i)$ be coordinates in $\mathbb{R}^d$ and let U denote a column vector of N fields. Consider the following initial value problem on this collection of fields

$$A\partial_0 U(x) + B^i\partial_i U(x) + CU(x) = 0 \tag{1.19}$$

$$U(0,x^i) = f(x^i) \tag{1.20}$$

where A, B^i and C are constant $N\times N$ matrices and $\det A \neq 0$. In this simple example, it is possible to find a formal solution by taking the spatial Fourier transform of (1.19). To see how this works, let

$$\tilde{U}(x^0,\xi_i) \equiv \frac{1}{(2\pi)^{(d-1)/2}}\int \mathrm{d}^{d-1}x\; e^{-i\xi_k x^k}U(x^0,x^i). \tag{1.21}$$

Then the Fourier transform of (1.19) can be written as

$$\partial_0 \tilde{U} = -A^{-1}\left(iB^k\xi_k + C\right)\tilde{U}. \tag{1.22}$$

For the sake of convenience, let us denote the matrix coefficient of $\tilde{U}$ appearing on the RHS of (1.22) by $i\mathcal{M}(\xi_i)$, i.e.

$$\mathcal{M}(\xi_i) \equiv A^{-1}\left(-B^k\xi_k + iC\right). \tag{1.23}$$

Now (1.22) can be directly integrated in x^0 to obtain a solution for the spatial Fourier transform of U in terms of the Fourier transform of the initial data that we shall denote by $\tilde{U}(0,\xi_i) = \tilde{f}(\xi_i)$. The solution is simply

$$\tilde{U}(x^0,\xi_i) = e^{i\mathcal{M}(\xi_i)x^0}\tilde{f}(\xi_i). \tag{1.24}$$

Taking the inverse Fourier transform of this yields the promised formal solution for the fields $U(x)$:

$$U(x) = \frac{1}{(2\pi)^{(d-1)/2}}\int \mathrm{d}^{d-1}\xi\; e^{i\xi_k x^k} e^{i\mathcal{M}(\xi_i)x^0}\tilde{f}(\xi_i). \tag{1.25}$$

The reason for emphasizing that (1.25) is merely a *formal* solution is that the integral may not be well-defined for a generic $\mathcal{M}(\xi_i)$. The problem of convergence of this integral comes down to the behaviour of the integrand at large wavenumbers, i.e. when $|\xi| \equiv \sqrt{\xi_i\xi_j\delta^{ij}} \to \infty$. (Note that we could use any other positive definite inverse metric to define the norm $|\cdot|$.) A simple sufficient condition that guarantees the existence of the solution (1.25) is the following: suppose there exists real constants $\Lambda > 0$ and λ such that the inequality

$$|e^{i\mathcal{M}(\xi_i)x^0}| \leq \Lambda e^{\lambda x^0} \tag{1.26}$$

holds for any covector ξ_i and for all time $x^0 \geq 0$.[4] Clearly, this implies that

$$|U(x)| \leq \Lambda e^{\lambda x^0}|f(x^i)| \tag{1.27}$$

or if the data $f(x^i)$ is $L^2(\mathbb{R}^{d-1})$ then

[4]Here the norm of the $N \times N$ matrix is defined in the usual way, i.e. as

$$|e^{i\mathcal{M}(\xi_i)x^0}| \equiv \sup_{U\in\mathbb{R}^N\setminus\{0\}} \frac{|e^{i\mathcal{M}(\xi_i)x^0}U|}{|U|}.$$

$$||U||_{L^2}(x^0) \leq \Lambda e^{\lambda x^0} ||f||_{L^2}. \tag{1.28}$$

This inequality tells us that the L^2 norm of the solution is controlled by the L^2 norm of the data, precisely the requirement needed for well-posedness.

Interestingly, it is possible to formulate the condition (1.26) in a different way. It can be shown [40] that the condition (1.26) is equivalent to the existence of a family of positive definite, uniformly bounded and Hermitian matrices $\mathcal{K}(\xi_i)$ (called the *Kreiss-symmetrizer* [40]) that satisfies

$$\mathcal{K}(\xi)i\mathcal{M}(\xi) - i\mathcal{M}(\xi)^\dagger \mathcal{K}(\xi) \leq 2\lambda \mathcal{K}(\xi) \qquad \text{and} \qquad \Lambda^{-1} I \leq \mathcal{K}(\xi_i) \leq \Lambda I. \tag{1.29}$$

for a positive constant Λ. To shed some light on the significance of the matrix $\mathcal{K}(\xi_i)$, we define an inner product (or "energy") using $\mathcal{K}(\xi_i)$ on solutions of (1.19) by

$$(U, V)_{\mathcal{K}}(x^0) \equiv \frac{1}{(2\pi)^{(d-1)/2}} \int \mathrm{d}^{d-1}x \int \mathrm{d}^{d-1}\xi \; e^{i\xi_k x^k} \tilde{U}(x^0, \xi_i)^\dagger \mathcal{K}(\xi_i) \tilde{V}(x^0, \xi_i). \tag{1.30}$$

This allows us to construct a positive, energy-like quantity that is quadratic in the fields U. A simple calculation [40] then reveals that the $\mathcal{K}$-norm of solutions of (1.19) satisfies

$$\partial_0 (U, U)_{\mathcal{K}}(x^0) \leq 2\lambda (U, U)_{\mathcal{K}}(x^0). \tag{1.31}$$

which implies (after an application of Gronwall's inequality) the following *energy estimate*

$$(U, U)_{\mathcal{K}}(x^0) \leq e^{2\lambda x^0} (f, f)_{\mathcal{K}}, \tag{1.32}$$

that is, the $\mathcal{K}$-energy of the solution at time x^0 is controlled by the $\mathcal{K}$-energy of the initial data. Note that the second inequality of (1.29) guarantees that the $\mathcal{K}$-energy is equivalent to the L_2-norm, and hence the solution satisfies (1.28).

Let us investigate the condition (1.26) a little further! As mentioned above, (1.26) ultimately constrains $\mathcal{M}(\xi_i)$ at large wavenumbers. To study the $|\xi| \to \infty$ limit, it is useful to rescale the variables x^0 and ξ by defining

$$\hat{t} \equiv \frac{x^0}{|\xi|} \qquad \text{and} \qquad \hat{\xi}_i \equiv \frac{\xi_i}{|\xi|}. \tag{1.33}$$

Now let us take the limit $|\xi| \to \infty$ on the LHS of (1.26) while keeping $\hat{t}$ fixed at some finite value. This gives us the inequality

$$|e^{iM(\hat{\xi}_i)\hat{t}}| \leq \Lambda \tag{1.34}$$

for the matrix $M(\hat{\xi}_i)$ defined by

$$M(\hat{\xi}_i) \equiv \lim_{|\xi|\to\infty} \frac{\mathcal{M}(\xi_i)}{|\xi|} = -A^{-1}B^i\hat{\xi}_i. \tag{1.35}$$

A simple argument reveals that the inequality (1.34) can only be satisfied if $M(\hat{\xi}_i)$ has only real eigenvalues. Suppose that the contrary is true. Then since $M(\hat{\xi}_i)$ is real, it must have a complex conjugate pair of eigenvalues κ and κ^*. Now consider the action of $\exp\left(iM(\hat{\xi}_i)\hat{t}\right)$ on the eigenvectors (normalised to 1) V and V^* corresponding to the eigenvalues κ and κ^*:

$$\begin{aligned} |e^{iM(\hat{\xi}_i)\hat{t}}V| &= e^{i\mathrm{Re}(\kappa)\hat{t}}e^{-\mathrm{Im}(\kappa)\hat{t}} \\ |e^{iM(\hat{\xi}_i)\hat{t}}V^*| &= e^{i\mathrm{Re}(\kappa*)\hat{t}}e^{-\mathrm{Im}(\kappa*)\hat{t}} = e^{i\mathrm{Re}(\kappa)\hat{t}}e^{\mathrm{Im}(\kappa)\hat{t}}. \end{aligned}$$

To avoid exponential growth in $\hat{t}$ (that may be arbitrarily large), we must have $\mathrm{Im}(\kappa) = 0$.

Even if $M(\hat{\xi}_i)$ has only real eigenvalues, it is not quite sufficient to satisfy (1.34): it also needs to be diagonalizable. For if there is a Jordan block of size $m \times m$ in the Jordan normal form of $M(\hat{\xi}_i)$ then $|\exp\left(iM(\hat{\xi}_i)\hat{t}\right)|$ may exhibit polynomial growth in $\hat{t}$ proportional to $|\hat{t}|^m$ [40]. This is an obstruction to derive an inequality of the form (1.28). However, it may be possible to obtain a weaker bound with a "loss of derivatives" of the form

$$||U||_{L^2}(x^0) \leq \Lambda e^{\lambda x^0} \sum_{|\alpha|\leq m} ||\partial^\alpha f||_{L^2}. \tag{1.36}$$

where α is a spatial multi-index. Similarly, the H^k-norm of the solution may only be bounded with the H^{k+m}-norm of the initial data. This means that if the initial data is $f \in H^s$ then this bound only guarantees the solution to be in H^{s-m}, i.e. the number of regular derivatives of the solution is fewer than that of the initial data (hence the term "loss of derivatives"). This type of bound may be acceptable for well-posedness in the case of constant coefficient linear equations but not for non-linear equations which is what we are ultimately interested in. Therefore, we shall require that $M(\hat{\xi}_i)$

is diagonalizable with real eigenvalues. It follows that $M(\hat{\xi}_i)$ can be decomposed as

$$M(\hat{\xi}_i) = S(\hat{\xi}_i)D(\hat{\xi}_i)S^{-1}(\hat{\xi}_i) \tag{1.37}$$

where D is diagonal and S denotes the matrix whose columns are the eigenvectors of $M(\hat{\xi}_i)$.

To see the connection between the diagonalizability of $M(\hat{\xi}_i)$ and the existence of $\mathcal{K}$, we define the matrix

$$\mathcal{K}'(\hat{\xi}_i) = \left(S^{-1}\right)^{\dagger}\left(S^{-1}\right). \tag{1.38}$$

This matrix is Hermitian and positive definite by construction. Furthermore, $M(\hat{\xi}_i)$ is Hermitian with respect to $\mathcal{K}'(\hat{\xi}_i)$, i.e., it satisfies

$$\mathcal{K}'(\hat{\xi}_i)M(\hat{\xi}_i)\mathcal{K}'(\hat{\xi}_i)^{-1} = M(\hat{\xi}_i)^{\dagger}. \tag{1.39}$$

The correspondence between the two formulations follows by noticing that (1.29) implies that setting $\mathcal{K}(\hat{\xi}_i) = \mathcal{K}'(\hat{\xi}_i)$ satisfies (1.39). Furthermore, if there exists a postive definite Hermitian matrix $\mathcal{K}(\xi_i)$ that satisfies (1.29) (and hence (1.39)) then $M(\hat{\xi}_i)$ is diagonalizable with real eigenvalues. A matrix $\mathcal{K}(\hat{\xi}_i)$ that satisfies these properties is called a *symmetrizer* of $M(\hat{\xi}_i)$.

The above observations motivate the following two notions of hyperbolicity. We say that the PDE (1.19) is *weakly hyperbolic* if the matrix $M(\hat{\xi}_i)$ defined in (1.35) has only real eigenvalues. The system (1.19) is called *strongly hyperbolic* if $M(\hat{\xi}_i)$ has a positive definite, Hermitian symmetrizer $\mathcal{K}$ that satisfies (1.39) and is uniformly bounded in the sense of the second inequality of (1.29).

As explained earlier, for weakly hyperbolic systems, we can only write down an energy estimate with loss of derivatives of the form (1.36), whereas for strongly hyperbolic systems, it is possible to bound the solutions in terms of the initial data without loss of derivatives. This difference matters crucially in the case of nonlinear systems of PDEs: if the linearization of the system is only weakly hyperbolic, then the estimates of the type (1.36) are not strong enough to establish the well-posedness of the nonlinear system. However, as explained in the next subsections, strong hyperbolicity is sufficient for the well-posedness of the nonlinear system.

1.2.3 Non-linear first order equations

Let us consider now a first-order *quasilinear* equation on $\mathbb{R}^d$ of the form

$$A(x,U)\partial_0 U + B^i(x,U)\partial_i U + C(x,U) = 0 \tag{1.40}$$

in a coordinate system $x^\mu = (x^0, x^i)$ where U is an N-component column vector, A, B and C are $N \times N$ matrix valued functions with smooth dependence on their arguments. We prescribe initial data

$$U(0,x^i) = f(x^i) \tag{1.41}$$

on the hypersurface $x^0 = 0$. We assume that constant time surfaces are *non-characteristic*, that is, $A(x,U)$ is invertible on these slices. Then equation (1.40) can be rewritten as

$$\partial_0 U = (B')^i(x,U)\partial_i U + C'(x,U) \tag{1.42}$$

with $(B')^i = -A^{-1}B^i$ and $C' = -A^{-1}C$. As illustrated in the previous subsection, hyperbolicity is an algebraic condition on the matrix $\mathcal{M}(x,U,\xi_i) \equiv (B')^i(x,U)\xi_i$ which contains information about the highest derivative (principal) terms in (1.40).

Definition 1.1. *Let ξ_i have unit norm w.r.t. a smooth positive definite (inverse) metric G^{ij} on surfaces of constant x^0. Equation* (1.40) *is* **weakly hyperbolic** *if all eigenvalues of $\mathcal{M}(x,U,\xi_i)$ are real for any such ξ_i. Equation* (1.40) *is* **strongly hyperbolic** *if there exists an $N \times N$ Hermitian matrix valued function $\mathcal{K}(x,U,\xi_i)$ (called the* **symmetrizer***) that is positive definite with smooth dependence on its arguments, and a positive constant Λ satisfying the conditions*

$$\mathcal{K}(x,U,\xi_i)\mathcal{M}(x,U,\xi_i) = \mathcal{M}^\dagger(x,U,\xi_i)\mathcal{K}(x,U,\xi_i) \tag{1.43}$$

and

$$\Lambda^{-1} I \leq \mathcal{K}(x,U,\xi_i) \leq \Lambda I. \tag{1.44}$$

The standard way to prove strong hyperbolicity is to show that $\mathcal{M}(x,U,\xi_i)$ is diagonalizable with real eigenvalues and a complete set of linearly independent and bounded eigenvectors that depend smoothly on the variables (x,U,ξ_i). Then one can use the eigenvectors to construct a suitable symmetrizer: if S denotes the matrix whose columns are the eigenvectors of $\mathcal{M}(x,U,\xi_i)$, then it is easy to check that $\mathcal{K} = (S^{-1})^\dagger S^{-1}$ is a positive definite, smooth and bounded symmetrizer (provided we restrict to a compact region of spacetime).

Let t be an eigenvector of $\mathcal{M}(x, U, \xi_i)$ with eigenvalue ξ_0. A different way of expressing this condition is

$$\left(A(x, U)\xi_0 + B^i(x, U)\xi_i\right) t = 0. \tag{1.45}$$

We can write this equation in a covariant way by introducing the covector $\xi_\mu = (\xi_0, \xi_i)$ and the vector $\mathcal{P}^\mu(x, U) = (A(x, U), B^i(x, U))$. Then (1.45) is equivalent to

$$\mathcal{P}^\mu(x, U)\xi_\mu t = 0. \tag{1.46}$$

Note that (1.46) is satisfied for some "polarization" t if $\det \mathcal{P}(x, U, \xi) = 0$. These observations motivate the following definition.

Definition 1.2. *Let ξ_μ be a general covector. We will refer to the $N \times N$ matrix*

$$\mathcal{P}(x, U, \xi) \equiv \mathcal{P}^\mu(x, U)\xi_\mu = A(x, U)\xi_0 + B^i(x, U)\xi_i$$

as the **principal symbol** *of equation* (1.40). *We say that the covector ξ_μ is* **characteristic** *if*

$$\det \mathcal{P}(x, U, \xi) = 0. \tag{1.47}$$

Similarly, let Σ be a codimension 1 hypersurface, specified by $h =$ constant where h is a smooth function $\mathbb{R}^d \to \mathbb{R}$ so that dh is nonzero on Σ. Then we say that Σ is a characteristic hypersurface if dh is a characteristic covector on Σ.

The principal symbol of (1.40) is obtained by selecting the first derivative (principal) terms in (1.40) and replacing the derivatives $\partial_\mu \equiv (\partial_0, \partial_i)$ by ξ_μ. It is also worth mentioning that a characteristic covector corresponds to the wavevector of an infinitely high frequency plane wave solution of (1.40) with polarization t.

Strong hyperbolicity can be similarly defined for first-order equations that are not quasilinear in the spatial derivatives, i.e. equations of the form

$$\partial_0 U = B(x, U, \partial_i U), \qquad U(0, x^i) = f(x^i). \tag{1.48}$$

In this case, the condition of strong hyperbolicity refers to the matrix

$$\mathcal{M}(x, U, \partial_i U, \xi_i) = (\partial_{\partial_j U} B)(x, U, \partial_i U)\xi_j \tag{1.49}$$

and the symmetrizer $\mathcal{K}(x, U, \partial_i U, \xi_i)$ must also depend smoothly on the spatial derivatives of U.

The following theorem relates strong hyperbolicity to the well-posedness of the initial value problem.

Theorem 1.2. *For strongly hyperbolic first order quasilinear systems* (1.40) *and nonquasilinear systems of the form* (1.48)*, the Cauchy problem with initial data* $U(0, x^i) = f(x^i)$ *is well-posed in Sobolev spaces* H^s *with* $s > s_0$ *for some constant* s_0*.*

In more detail, let $C^0([0, T), H^s(\mathbb{R}^{d-1}))$ *denote the space of* C^0 *functions* $[0, T) \to H^s(\mathbb{R}^{d-1})$*, i.e. the space of functions* U *satisfying*

$$\lim_{t_k \to t_0} ||U(t_k, x) - U(t_0, x)||_{H^s} = 0$$

for any sequence $\{t_k\} \subset [0, T)$ *approaching* $t_0 \in [0, T)$*. Furthermore, let the initial data be* $f \in H^s(\mathbb{R}^{d-1})$*. Then there exists a unique local solution to* (1.48) *with* $U \in C^0([0, T), H^s(\mathbb{R}^{d-1}))$ *and* $T > 0$ *depends on the* H^s*-norm of the initial data.*

The theorem above is proved in e.g. Chapter 5 of [41][5]. The statements about the quasilinear and the nonquasilinear systems differ only in the required order of regularity for the initial data, i.e. the value of s_0. However, we shall not be concerned with the problem of optimal regularity in this thesis.

1.2.4 Second order equations

Let $x^\mu = (x^0, x^i)$ be coordinates in a d-dimensional spacetime. Consider a set of fields u_I, $I = 1, \ldots, N$ satisfying a second order PDE

$$V^I(x, u, \partial u, \partial^2 u) = 0 \tag{1.50}$$

with initial conditions

$$u(0, x^i) = f(x^i), \qquad \partial_0 u(0, x^i) = g(x^i) \tag{1.51}$$

We do not assume that the equation is quasilinear. We define the *principal symbol* as

$$\mathcal{P}(\xi)^{IJ} \equiv \mathcal{P}^{IJ\mu\nu}\xi_\mu\xi_\nu \equiv \frac{\partial V^I}{\partial(\partial_\mu\partial_\nu u_J)}\xi_\mu\xi_\nu. \tag{1.52}$$

[5]Note in this reference strong hyperbolicity is called symmetrizable hyperbolicity.

Suppressing the IJ indices we have

$$\mathcal{P}(\xi) = \mathcal{P}^{\mu\nu}\xi_\mu\xi_\nu = \xi_0^2 A + \xi_0 B(\xi_i) + C(\xi_i) \tag{1.53}$$

where the $N \times N$ matrices A, B, C are given by

$$A = \mathcal{P}^{00}, \qquad B(\xi_i) = 2\mathcal{P}^{0i}\xi_i, \qquad C(\xi_i) = \mathcal{P}^{ij}\xi_i\xi_j \tag{1.54}$$

These matrices depend on $x, u, \partial u$ and $\partial^2 u$ although we will not write this explicitly. *We will restrict attention to equations for which V^I depends linearly on $\partial_0^2 u$.* This implies that

$$V^I(x,u,\partial u,\partial^2 u) = A^{IJ}(x,u,\partial u,\partial_0\partial_i u,\partial_i\partial_j u)\partial_0^2 u_J + W^I(x,u,\partial u,\partial_0\partial_i u,\partial_i\partial_j u). \tag{1.55}$$

We also assume that $x^0 = 0$ is non-characteristic, which means that initial data (1.51) is chosen so that $\det A \neq 0$ at $x^0 = 0$. By continuity, this condition will continue to hold in a neighbourhood of $x^0 = 0$. We can then rewrite the equation as

$$\partial_0^2 u_I = X_I(x,u,\partial u,\partial_0\partial_i u,\partial_i\partial_j u) \tag{1.56}$$

where

$$X_I = -(A^{-1})_{IJ}W^J. \tag{1.57}$$

Note that

$$\begin{aligned}
\frac{\partial X_I}{\partial(\partial_i\partial_j u_J)} &= -(A^{-1})_{IK}\frac{\partial W^K}{\partial(\partial_i\partial_j u_J)} + (A^{-1})_{IK}\frac{\partial A^{KL}}{\partial(\partial_i\partial_j u_J)}(A^{-1})_{LM}W^M \\
&= -(A^{-1})_{IK}\left[\frac{\partial W^K}{\partial(\partial_i\partial_j u_J)} + \frac{\partial A^{KL}}{\partial(\partial_i\partial_j u_J)}\partial_0^2 u_L\right] = -(A^{-1})_{IK}\frac{\partial V^K}{\partial(\partial_i\partial_j u_J)} \\
&= -(A^{-1})_{IK}\mathcal{P}^{KJij}
\end{aligned} \tag{1.58}$$

where we used the equation of motion (1.56) in the second equality. Similarly[6]

$$\frac{\partial X_I}{\partial(\partial_0\partial_i u_J)} = -2(A^{-1})_{IK}\mathcal{P}^{KJ0i}. \tag{1.59}$$

[6] The factor of 2 can be understood by varying $\partial_\mu\partial_\nu u$ in (1.55). On the LHS this gives $\mathcal{P}^{\mu\nu}\delta(\partial_\mu\partial_\nu u)$ which, by the symmetry of mixed partial derivatives, contains a term $2\mathcal{P}^{0i}\delta(\partial_0\partial_i u)$.

We will now write the second order system (1.56) as a first order system. Define $v_0 \equiv \partial_0 u$ and $v_i \equiv \partial_i u$. Then (1.56) implies[7]

$$\begin{aligned} \partial_0 u &= v_0 \\ \partial_0 v_i &= \partial_i v_0 \\ \partial_0 v_0 &= X(x, u, v, \partial_i v_0, \partial_i v_j) \end{aligned} \tag{1.60}$$

together with the constraint equations $\mathcal{C}_i = 0$ where

$$\mathcal{C}_i \equiv v_i - \partial_i u. \tag{1.61}$$

The evolution system (1.60) is of the form (1.48) with the variable $U \equiv (u, v_i, v_0)$. Initial data for the auxiliary variable v_i can be constructed from the data (1.51) by taking the spatial derivatives of the data for u on the initial surface. Hence the initial data for U is

$$U(0, x^j) = \left(f(x^j), \partial_i f(x^j), g(x^j)\right). \tag{1.62}$$

Note in particular that by construction this data satisfies the constraint equation. Then it follows from the equations (1.60) that the constraints will also be satisfied at later times. To see this, take a time derivative of (1.61) which gives

$$\partial_0 \mathcal{C}_i = \partial_0 v_i - \partial_0 \partial_i u = \partial_0 v_i - \partial_i v_0 = 0. \tag{1.63}$$

It follows that if (u, v_0, v_i) is a solution of (1.60) arising from initial data of the form (1.62) then u will be a solution of (1.56) satisfying the initial conditions (1.51).

We will now demand that the first order system (1.60) is strongly hyperbolic and determine the conditions that this imposes on the second order system that we started from. The matrix $\mathcal{M}$ defined in (1.49) is

$$\mathcal{M} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \xi_i \\ 0 & \frac{\partial X_I}{\partial(\partial_i(v_j)_J)}\xi_i & \frac{\partial X_I}{\partial(\partial_i(v_0)_J)}\xi_i \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \xi_i \\ 0 & -(A^{-1})_{IK}\mathcal{P}^{KJij}\xi_i & -(A^{-1})_{IK}B^{KJ} \end{pmatrix} \tag{1.64}$$

[7]Note that one could have considered a more general way of reducing the second order system to a first order one (i.e. the variables v_0 and v_i could be defined as more complicated linear combinations of the first derivatives of u). Although it is reasonable to expect that the derivation presented in this section would not depend on the details of such (more general) reductions, we will not investigate this problem here.

in the second equality we used $\partial X/(\partial(\partial_i v_j)) = \partial X/(\partial(\partial_i\partial_j u))$ and equation (1.58), $\partial X/(\partial(\partial_i v_0)) = \partial X/(\partial(\partial_0\partial_i u))$ and equation (1.59), and the definition of B^{IJ}.

This matrix acts on a vector space of dimension $(d+1)N$. A general vector in this space can be written $(s_J, (t_i)_J, (t_0)_J)$. The definition of strong hyperbolicity of the first order system refers to a smooth Riemannian (inverse) metric G^{ij} on surfaces of constant x^0. It is convenient to separate $(t_i)_J$ into a part $(t_i^\perp)_J$ perpendicular to ξ_i w.r.t. G^{ij}, and a part $t_J^\parallel \xi_i$ parallel to ξ_i. We then order the components of our vector as $(s_J, (t_i^\perp)_J, t_J^\parallel, (t_0)_J)$. With this decomposition, $\mathcal{M}$ becomes

$$\mathcal{M} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & I \\ 0 & -(A^{-1})_{IK}(\mathcal{P}^{KJij}\xi_i)^\perp & -(A^{-1})_{IK}C^{KJ} & -(A^{-1})_{IK}B^{KJ} \end{pmatrix} \tag{1.65}$$

where I is the $N \times N$ identity matrix and $(\mathcal{P}^{KJij}\xi_i)^\perp$ is the restriction of $\mathcal{P}^{KJij}\xi_i$ to vectors of the form $(t_i^\perp)_J$.

We write a general vector as the sum of $(s_J, (t_i^\perp)_J, 0, 0)$ and $(0, 0, t_J^\parallel, (t_0)_J)$ respectively. This gives a block decomposition of $\mathcal{M}$

$$\mathcal{M} = \begin{pmatrix} 0 & 0 \\ L & M \end{pmatrix} \tag{1.66}$$

where L is the $2N \times (d-1)N$ matrix

$$L = \begin{pmatrix} 0 & 0 \\ 0 & -(A^{-1})_{IK}(\mathcal{P}^{KJij}\xi_i)^\perp \end{pmatrix} \tag{1.67}$$

and M is the $2N \times 2N$ matrix

$$M = \begin{pmatrix} 0 & I \\ -A^{-1}C & -A^{-1}B \end{pmatrix}. \tag{1.68}$$

The matrices L and M (and hence $\mathcal{M}$) depend on $(x, u, \partial u, \partial_0\partial_i u, \partial_i\partial_j u, \xi_i)$, or equivalently on $(x, u, v, \partial_i v, \xi_i)$.

We now examine the conditions for our first order system to admit a symmetrizer. Any Hermitian $(d+1)N \times (d+1)N$ matrix $\mathcal{K}$ can be written as

$$\mathcal{K} = \begin{pmatrix} E & F \\ F^\dagger & K \end{pmatrix} \tag{1.69}$$

where E is a $(d-1)N \times (d-1)N$ Hermitian matrix, K is a $2N \times 2N$ Hermitian matrix and F is a $(d-1)N \times 2N$ matrix. Equation (1.43) reduces to

$$KM = M^\dagger K \tag{1.70}$$

and

$$FL = (FL)^\dagger \qquad\qquad FM = L^\dagger K \tag{1.71}$$

Let us assume that we can find a positive definite Hermitian matrix K, depending smoothly on $(x, u, v, \partial_i v, \xi_i)$, and satisfying (1.70) and $\lambda^{-1} I \leq K \leq \lambda I$ for some positive constant λ. Assume also that M is invertible. We can then satisfy (1.71) with $F = L^\dagger K M^{-1}$. We then take $E = cI$ where c is a positive constant. Let $T \equiv (T_1, T_2)^\dagger$ with $T_1 \equiv (s_J, (t_i^\perp)_J)^\dagger$ and $T_2 \equiv (t_J^\parallel, (t_0)_J)^\dagger$ and consider

$$T^\dagger \mathcal{K} T = cT_1^\dagger T_1 + T_1^\dagger F T_2 + T_2^\dagger F^\dagger T_1 + T_2^\dagger K T_2. \tag{1.72}$$

If $\mathcal{P}^{IJ\mu\nu}$ is uniformly bounded then so are the matrices M, L and F when ξ_i is a unit covector w.r.t. a positive definite (inverse) metric G^{ij}. By taking c large enough we can ensure that $\mathcal{K}$ is positive definite and (1.44) holds for some Λ. Hence we have constructed a symmetrizer for the first-order system.

This motivates the following definitions for our second order equation:

Definition 1.3. *Consider a second order PDE* (1.50) *satisfying* (1.55)*. Define the matrix M, depending on $(x, u, \partial u, \partial_0 \partial_i u, \partial_i \partial_j u, \xi_i)$, by* (1.68)*. Let ξ_i have unit norm w.r.t. a smooth positive definite (inverse) metric G^{ij} on surfaces of constant x^0. The equation is* **weakly hyperbolic** *if all eigenvalues of M are real for any such ξ_i. The equation is* **strongly hyperbolic** *if there exists a $2N \times 2N$ Hermitian matrix valued function $K(x, u, \partial u, \partial_0 \partial_i u, \partial_i \partial_j u, \xi_i)$ (called the* **symmetrizer***) that is positive definite with smooth dependence on its arguments, and that satisfies* (1.70)*, and a positive constant λ such that $\lambda^{-1} I \leq K \leq \lambda I$.*

Note that any eigenvalue of $\mathcal{M}$ is either 0 or an eigenvalue of M. Hence if our second order PDE is weakly hyperbolic according to the above definition, then the first-order system (1.60) is weakly hyperbolic according to our previous definition. If our second order PDE is strongly hyperbolic according to the above definition and M is also invertible, then the above discussion shows that we can construct a symmetrizer for the first-order system (1.60) and so this system is also strongly hyperbolic. Hence we can apply the well-posedness theorem stated at the end of the previous section to deduce the well-posedness of the initial value problem for the second-order system.

The condition that M should be invertible was used above, but it is not a necessary condition for well-posedness. However, if this condition is not satisfied, then it may be necessary to explore different ways of reducing the second-order equation to a first-order system (see section 1.2.5). This condition is equivalent to the condition that C should be invertible. (This is also equivalent to the condition that $(0, \xi_i)$ is never characteristic (see Definition 1.4), which is equivalent to the condition that $\xi_0 \neq 0$ for any characteristic covector ξ_μ.)

We conclude this section by extending the definition of characteristic covectors and hypersurfaces to second order PDEs.

Definition 1.4. *We say that a covector ξ_μ is a characteristic covector of* (1.50) *if it satisfies*

$$\det \mathcal{P}(\xi) = 0 \tag{1.73}$$

where $\mathcal{P}(\xi)$ is the principal symbol defined in (1.52). *Similarly, a codimension* 1 *hypersurface Σ given by $h =$ constant (where h is a smooth function $\mathbb{R}^d \to \mathbb{R}$ with $dh \neq 0$ on Σ) is said to be characteristic if dh is a characteristic covector on Σ.*

Suppose that ξ_μ is a characteristic covector of equation (1.50). Then there exists a "polarization" t (i.e. an N-component column vector) satisfying

$$\mathcal{P}(\xi)t = \left(\xi_0^2 A + \xi_0 B(\xi_i) + C(\xi_i)\right) t = 0. \tag{1.74}$$

It is easy to check that this equation implies that $(t, \xi_0 t)^T$ is an eigenvector of $M(\xi_i)$ with eigenvalue ξ_0. Equivalently, eigenvectors of $M(\xi_i)$ corresponding to eigenvalue ξ_0 must have the form $(t, \xi_0 t)^T$ where t satisfies (1.74) and the covector $\xi_\mu = (\xi_0, \xi_i)$ is characteristic. This shows that one can establish strong hyperbolicity of the second order PDE system (1.50) by finding the characteristic covectors of (1.50) and the corresponding polarizations.

1.2.5 Partially reduced second order systems

When discussing numerical-relativity-inspired formulations of the Einstein equations, we will encounter systems of PDEs that are first order in time derivatives but are second order in spatial derivatives of some of the variables. These systems are obtained by only partially reducing a second-order PDE system to a first-order one.

To make it clearer what is meant by this, we consider a set of n fields represented by the n- component column vector valued function u and another set of m fields represented by the m- component column vector valued function v. Assume these fields satisfy the system of $n+m$ PDEs

$$\begin{aligned} \partial_0 u &= M^k_{uu}(x,u)\partial_k u + M_{uv}(x)v \qquad (1.75)\\ 0 &= V(x,u,\partial_i u,\partial_i\partial_j u,\partial_0 v,\partial_i v) \qquad (1.76)\end{aligned}$$

where $\{M^k_{uu}\}^{d-1}_{k=1}$ are $n\times n$ matrices, M_{uv} is an $n\times m$ matrix and V is an m-component column vector valued function. We can think about the fields v as a combination of first derivatives of the fields u. Similarly to the previous subsection, we assume that V depends linearly on $\partial_0 v$, i.e.

$$V(x,u,\partial_i u,\partial_i\partial_j u,\partial_0 v,\partial_i v) = A_{vv}(x,u,\partial_i u,\partial_i\partial_j u,\partial_i v)\partial_0 v + W(x,u,\partial_i u,\partial_i\partial_j u,\partial_i v). \qquad (1.77)$$

where A_{vv} is an $m\times m$ matrix valued function. We place initial data

$$u(0,x^i) = f(x^i), \qquad v(0,x^i) = g(x^i) \qquad (1.78)$$

on a non-characteristic surface $x^0=0$ so that the matrix A_{vv} is invertible at $x^0=0$ and in its neighbourhood. This allows us to write the system as

$$\begin{aligned} \partial_0 u &= M^k_{uu}(x,u)\partial_k u + M_{uv}(x,u)v\\ \partial_0 v &= X(x,u,\partial_i u,\partial_i\partial_j u,\partial_i v) \qquad (1.79)\end{aligned}$$

with $X \equiv -A^{-1}_{vv}W$. To rewrite (1.79) as a proper first order system, we can repeat the approach of the previous subsection and introduce the auxiliary variable $v_i \equiv \partial_i u$. Then we have a larger system for the $n(d+1)+m$ variables (u,v,v_i):

$$
\begin{aligned}
\partial_0 u &= M^k_{uu}(x,u)\partial_k u + M_{uv}(x,u)v \\
\partial_0 v &= X(x,u,\partial_i u,\partial_i\partial_j u,\partial_i v) \\
\partial_0 v_i &= \partial_i\left(M^k_{uu}(x,u)v_k\right) + \partial_i\left(M_{uv}(x,u)v\right)
\end{aligned}
\tag{1.80}
$$

where the initial data for v_i is just $\partial_i f$. The system (1.80) must be complemented with the extra constraint equation $\mathcal{C}_i = 0$ for the constraint variable $\mathcal{C}_i \equiv v_i - \partial_i u$. It follows from (1.80) that $\mathcal{C}_i$ satisfies $\partial_0 \mathcal{C}_i = 0$. Since $C_i = 0$ initially, it follows that the constraints are propagated and if (u, v, v_i) is a solution to (1.80) then (u, v) is a solution to (1.79). In this sense the two systems are equivalent.

Once again, we seek a condition for the enlarged system (1.80) to be strongly hyperbolic. We define the matrices

$$
M^{ij}_{vu} \equiv \frac{\partial X}{\partial(\partial_i\partial_j u)} \qquad \text{and} \qquad M^i_{vv} \equiv \frac{\partial X}{\partial(\partial_i v)} \tag{1.81}
$$

where the sizes of the matrices M^{ij}_{vu} are $m \times n$, the matrices M^i_{vv} are $m \times m$ and their dependence on $(x, u, \partial_i u, \partial_i\partial_j u, \partial_i v)$ is suppressed for simplicity. The matrix $\mathcal{M}$ defined in (1.49) corresponding to the first order system (1.80) is

$$
\mathcal{M}(\xi)\begin{pmatrix} t \\ s \\ s_i \end{pmatrix} \equiv \begin{pmatrix} 0 & 0 & 0 \\ 0 & M^k_{vv}\xi_k & M^{kj}_{vu}\xi_k \\ 0 & \xi_i M_{uv} & \xi_i M^j_{uu} \end{pmatrix}\begin{pmatrix} t \\ s \\ s_j \end{pmatrix} \tag{1.82}
$$

where t, s and s_i are column vectors of size n, m and md, respectively. We are going to show that the hyperbolicity of this system can be reduced to studying the eigenvalue problem of a smaller matrix under the right conditions. Suppose that the matrix

$$
M(\xi)\begin{pmatrix} u \\ v \end{pmatrix} \equiv \begin{pmatrix} M^k_{uu}\xi_k & M_{uv} \\ M^{kl}_{vu}\xi_k\xi_l & M^k_{vv}\xi_k \end{pmatrix}\begin{pmatrix} u \\ v \end{pmatrix} \tag{1.83}
$$

is diagonalizable with real eigenvalues and a complete set of $n+m$ linearly independent, bounded eigenvectors that depend smoothly on ξ_i. Then we claim that the system (1.80) is strongly hyperbolic.

To see that this is true, we demonstrate that under the above assumptions, the matrix (1.82) is diagonalizable with real eigenvalues. Consider an eigenvalue ξ_0 of (1.83) and an eigenvector $(t, s)^T$. Then it follows that $(0, s, \xi_i t)^T$ is an eigenvector of (1.82) with the same eigenvalue. This is clearly true for any of the $n+m$ eigenvalues and eigenvectors of (1.83). Hence, it remains to find nd additional eigenvalues and eigenvectors. It is easy to see that for an arbitrary choice of t, the vector $(t,0,0)^T$ is an eigenvector of (1.82) with eigenvalue $\xi_0 = 0$. Choosing a basis of vectors for the t slot gives n linearly independent eigenvectors. Finally, we can find an additional set of $n(d-1)$ eigenvectors corresponding to zero eigenvalue by solving the system of $n+m$ independent linear equations

$$\begin{pmatrix} M^i_{uu} & M_{uv} \\ M^{ki}_{vu}\xi_k & M^k_{vv}\xi_k \end{pmatrix} \begin{pmatrix} s_i \\ s \end{pmatrix} = 0 \tag{1.84}$$

for the $nd+m$ variables (s_i, s). Now assume that the matrix

$$\begin{pmatrix} M^i_{uu} & M_{uv} \\ M^{ki}_{vu}\xi_k & M^k_{vv}\xi_k \end{pmatrix} \tag{1.85}$$

has rank $n+m-p$ for some $p \geq 0$. This means that there exist p row vectors of the form (t,s) with $n+m$ components that satisfy

$$(t,s) \begin{pmatrix} M^i_{uu} & M_{uv} \\ M^{ki}_{vu}\xi_k & M^k_{vv}\xi_k \end{pmatrix} = 0 \tag{1.86}$$

which also implies

$$(t,s) \begin{pmatrix} M^i_{uu}\xi_i & M_{uv} \\ M^{ki}_{vu}\xi_k\xi_i & M^k_{vv}\xi_k \end{pmatrix} = (t,s)M(\xi_i) = 0. \tag{1.87}$$

This means that the matrix $M(\xi_i)$ defined in (1.83) has p left eigenvectors with 0 eigenvalue and hence it must have p-dimensional space of right eigenvectors with 0 eigenvalue. Since the matrix (1.85) has rank $n+m-p$ by assumption, it follows that the equations (1.84) have $(nd+m)-(n+m-p) = n(d-1)+p$ independent solutions for the variables (s_i, s). As just explained, p of this solutions must be of the form $(\xi_i t, s)$, corresponding to eigenvectors of $M(\xi_i)$ with zero eigenvalue. We have already accounted for these eigenvectors above. The remaining $n(d-1)$ solutions give rise to the $n(d-1)$ eigenvectors of $\mathcal{M}(\xi_i)$ promised above (1.84).

Strong hyperbolicity then follows from the argument explained under Definition 1.1: the symmetrizer can be constructed from the eigenvectors listed above.

To conclude this section, we mention that there is another way of expressing the eigenvalue problem of (1.83). Let us define the matrices

$$\mathbb{A} = \begin{pmatrix} I_{n\times n} & 0 \\ 0 & A_{vv} \end{pmatrix} \qquad \text{and} \qquad \mathbb{L}(\xi_i) = \begin{pmatrix} M^i_{uu}\xi_i & M_{uv} \\ \frac{\partial V}{\partial(\partial_k \partial_i u)}\xi_k\xi_i & \frac{\partial V}{\partial(\partial_k v)}\xi_k \end{pmatrix} \tag{1.88}$$

where $I_{n\times n}$ is the $n \times n$ unit matrix. Then using the identities (c.f. equations (1.58) and (1.59))

$$M^{ij}_{vu} = \frac{\partial X}{\partial(\partial_i \partial_j u)} = -A^{-1}_{vv}\frac{\partial V}{\partial(\partial_i \partial_j u)} \tag{1.89}$$

$$M^{i}_{vv} = \frac{\partial X}{\partial(\partial_i v)} = -A^{-1}_{vv}\frac{\partial V}{\partial(\partial_i v)} \tag{1.90}$$

we can write the eigenvalue problem of $M(\xi_i)$ as

$$\left(-\xi_0\mathbb{A} + \mathbb{L}(\xi_i)\right) U = 0 \tag{1.91}$$

where the column vector $U = (t, s)^T$ has $n + m$ components. This equation may be interpreted as the characteristic equation of the generalized principal symbol $\mathcal{P}(\xi) \equiv \xi_0\mathbb{A} - \mathbb{L}(\xi_i)$. Using this generalized notion, the "principal" terms in equation (1.75) are those involving first derivatives of u and terms involving v, whereas the principal terms in (1.76) are those involving second derivatives of u and first derivatives of v. In other words, the principal terms in a system of PDEs are the "least regular" terms.

1.3 The initial value problem in theories of gravity

1.3.1 General relativity

As explained in the previous section, the standard way to establish the local well-posedness of the initial value problem for a system of PDEs is to demonstrate that it is strongly hyperbolic. In a coordinate chart, Einstein's equation (1.1) is a coupled system of second order quasilinear PDEs for the components of the spacetime metric $g_{\mu\nu}$. For example, in vacuum, the system can be written as

$$-\frac{1}{2}P^{\mu\nu\rho\sigma}g^{\gamma\delta}\partial_\gamma\partial_\delta g_{\rho\sigma} + P_\alpha{}^{\gamma\mu\nu}g^{\alpha\beta}P_\beta{}^{\delta\rho\sigma}\partial_\gamma\partial_\delta g_{\rho\sigma} + \mathcal{F}^{\mu\nu}(g, \partial g) = 0 \tag{1.92}$$

where $\mathcal{F}$ is a function containing the terms with lower than second derivatives of g and

$$P_\alpha{}^{\beta\mu\nu} \equiv \delta_\alpha^{(\mu} g^{\nu)\beta} - \frac{1}{2}\delta_\alpha^\beta g^{\mu\nu}. \tag{1.93}$$

In a four-dimensional spacetime M, we need to prescribe initial data on a three-dimensional Cauchy-surface Σ. Assume that Σ is spacelike and let n denote the future-directed unit vector field normal to Σ. Hence, initial data for Einstein's equation is the triple (Σ, h_{ij}, K_{ij}) where h_{ij} and K_{ij} are the components of a Riemannian metric and a symmetric tensor on Σ, respectively. The metric h_{ij} corresponds to the initial data for the induced metric on Σ, K_{ij} is the initial data for the extrinsic curvature of Σ.

The system (1.92) is not strongly hyperbolic due to the diffeomorphism-covariance of the theory. This makes the discussion of the initial value problem in theories of gravity a bit more involved. Solving this problem requires finding a "good" gauge and a good way of fixing the gauge, i.e. Einstein's equation needs to be modified by terms that vanish when the gauge condition is satisfied. Then the general strategy to establish well-posedness for a gravitational theory consists of the following three steps.

1) Starting from initial data (Σ, h_{ij}, K_{ij}) in any coordinate system, we need to show that there exists a diffeomorphism such that the gauge condition is satisfied on Σ.

2) The next step is to show that the gauge condition is propagated. This means that solutions of the gauge-fixed e.o.m. arising from initial data that satisfies the gauge condition must also be solutions of the original e.o.m. (i.e. the equations without gauge-fixing).

3) The gauge-fixed system of equations is strongly hyperbolic.

In this section, we will not give a detailed discussion of how to implement this strategy. The first two steps will be carried out later in Chapter 3 in a more general setting. Instead, we continue with a brief discussion of the seminal work of Choquet-Bruhat [49] that was later extended [50,51] to prove the existence of a unique (up to diffeomorphisms) maximal globally hyperbolic development of a general Cauchy data. Here we only focus on the elegant harmonic gauge condition and the corresponding gauge-fixing procedure, and demonstrate that the gauge-fixed Einstein equations are strongly hyperbolic (i.e. step 3) above is satisfied).

Introducing

$$H^{\mu} \equiv g^{\nu\rho}\nabla_{\nu}\nabla_{\rho}x^{\mu} = -g^{\nu\rho}\Gamma^{\mu}_{\nu\rho}[g], \tag{1.94}$$

the harmonic gauge condition is simply

$$H^{\mu} = 0. \tag{1.95}$$

The gauge-fixing of the Einstein equations can be carried out by writing

$$G^{\mu\nu} + P_{\alpha}{}^{\beta\mu\nu}\partial_{\beta}H^{\alpha} = 0. \tag{1.96}$$

Equivalently, one can take the trace-reversed version of (1.96) to obtain a system of quasilinear wave equations[8]

$$R_{\mu\nu} + 2\partial_{(\mu}H_{\nu)} = -\frac{1}{2}g^{\alpha\beta}\partial_{\alpha}\partial_{\beta}g_{\mu\nu} + \mathcal{N}_{\mu\nu}(g, \partial g) = 0 \tag{1.97}$$

where the function $\mathcal{N}_{\mu\nu}$ encapsulates all the lower order terms in the equation.

The proof of strong hyperbolicity of (1.97) is quite simple, based on section 1.2.4 (see also [52]). Consider a coordinate system $\{x^{\mu}\}$ such that hypersurfaces of $x^0 =$ constant are spacelike. In particular, this implies that $g^{00} < 0$. For a general covector ξ_{μ}, the principal symbol of (1.97), acting on a symmetric tensor $t_{\alpha\beta}$ is

$$\mathcal{P}(\xi)_{\mu\nu}{}^{\alpha\beta}t_{\alpha\beta} = -\frac{1}{2}g^{\gamma\delta}\xi_{\gamma}\xi_{\delta}t_{\mu\nu}. \tag{1.98}$$

It follows that ξ_{μ} is characteristic if and only if it is null w.r.t. the metric g. Writing out this condition in our coordinate system gives a quadratic equation for the component ξ_0, provided that we fix the components ξ_i. Since $g^{00} \neq 0$ by assumption, this quadratic equation has two distinct, real and nonzero solutions for ξ_0 that we shall denote by $\xi_0^{\pm}$. Similarly, let $\xi_{\mu}^{\pm} = (\xi_0^{\pm}, \xi_i)$ denote the two families of characteristic covectors. Furthermore, we have $\mathcal{P}(\xi^{\pm})_{\mu\nu}{}^{\alpha\beta}t_{\alpha\beta} = 0$ for any symmetric tensor $t_{\alpha\beta}$. Strong hyperbolicity now follows from the discussion of section 1.2.4. The matrix $M(\xi_i)$ introduced in (1.35) is a 20×20 matrix (in 4 dimensions) acting on pairs of

[8] In most references the gauge-fixed Einstein equation is written as in equation (1.97) because it looks simpler than (1.96). However, in chapter 3, it will be more convenient to carry out the gauge-fixing of $G_{\mu\nu} = 0$. The reason for this is that this equation is directly obtained by varying the action which ensures that the principal symbol has certain symmetries. Exploiting these symmetries simplifies the analysis of chapter 3, especially for Lovelock and Horndeski theories. Note that taking any invertible linear combination of a system of PDEs does not change the hyperbolicity of the system so using the trace-reversed version of the equations should not make a difference in practice.

symmetric tensors $(t_{\mu\nu}, s_{\mu\nu})$. This matrix is diagonalizable with real eigenvalues: it has 10-dimensional degenerate eigenspace corresponding to the eigenvalue ξ_0^+ spanned by eigenvectors of the form $(t_{\mu\nu}, \xi_0^+ t_{\mu\nu})^T$ and similarly, a 10-dimensional degenerate eigenspace with eigenvalue ξ_0^- spanned by eigenvectors of the form $(t_{\mu\nu}, \xi_0^+ t_{\mu\nu})^T$. One can select a basis of eigenvectors in both eigenspaces that are bounded and have smooth dependence on ξ_i. A smooth and bounded symmetrizer can then be constructed using these eigenvectors, as described in section 1.2.1.

Note that not all mode solutions of the characteristic equation $\mathcal{P}(\xi)_{\mu\nu}{}^{\alpha\beta} t_{\alpha\beta} = 0$ are "physical" polarizations. Indeed, in 4 dimensions, a graviton has only two degrees of freedom. We can identify two types of "unphysical" mode solutions. The first type of such solutions violate the high frequency version of the harmonic gauge condition

$$\xi^\mu t_{\mu\nu} - \frac{1}{2}\xi_\nu g^{\mu\nu} t_{\mu\nu} = 0. \tag{1.99}$$

These "gauge-condition violating" solutions of the gauge-fixed equations are not solutions of the original (i.e. non-gauge-fixed) equations. The second type of unphysical solutions have the form

$$t_{\mu\nu} = \xi_{(\mu} Y_{\nu)} \tag{1.100}$$

where Y_ν is a general covector. When ξ_μ is characteristic (i.e. null), (1.100) satisfies (1.99) for any Y_ν. Since (1.100) has the form of the high frequency limit of an infinitesimal diffeomorphism generated by Y, we will refer to such polarizations as "pure gauge". Pure gauge modes are associated with residual gauge freedom.

Using the harmonic gauge provides a simple and elegant way to rewrite Einstein's equation in a strongly hyperbolic form. However, this is by no means the only good approach. Some alternative (locally) well-posed formulations will be presented in the upcoming chapters.

1.3.2 The initial value problem in modifications of general relativity

The initial value problem in modifications of general relativity has received much attention, particularly in recent years [44, 53–70].

As mentioned before, from an EFT perspective, the weakly coupled regime is the only situation in which we would trust EGB or 4∂ST theory because once the theory becomes strongly coupled, all of the higher derivative terms that we have neglected would become important. There are other reasons for restricting to the weakly coupled regime. Previous work has shown that even *weak* hyperbolicity can fail in Lovelock [59] or Horndeski [60, 62–66, 71–73] theories once the spacetime curvature and/or scalar field derivatives become large enough that the higher-derivative Lovelock or Horndeski terms in the equation of motion are comparable to the 2-derivative terms, i.e. in the strongly coupled regime. So in this regime, these theories are not expected to be viable as classical theories. Note, however, that weak couplings are compatible with the fields being strong in the sense of nonlinearities being important, e.g. it is compatible with black hole formation provided the black hole is large compared to, say, the length scale defined by the coupling constant k_2 in EGB theory.

Even at weak coupling, we still have to face the challenge of choosing a good gauge and fixing it appropriately. The hyperbolicity of the Lovelock and Horndeski equations of motion in a class of generalized harmonic gauge conditions have been investigated in [60, 61]. It was shown that, at weak coupling, these theories are weakly hyperbolic in such gauges. However, for Lovelock theories they are not strongly hyperbolic at weak coupling unless $k_p = 0$ for all p. Only a small subset of harmonic gauge Horndeski theories are strongly hyperbolic at weak coupling [60, 61]: the so-called k-essence theories. These can be obtained from the general Horndeski action by setting $G_3 = G_5 = 0$ and $\partial_X G_4 = 0$.

To briefly explain the failure of harmonic gauge in general Lovelock and Horndeski theories, let us go back to the harmonic gauge Einstein equation. In this gauge, the metric satisfies a nonlinear wave equation whose characteristic covectors are null with respect to the spacetime metric. In other words, the eigenvalues of the matrix $M(\xi_i)$ relevant for strong hyperbolicity have highly degenerate eigenvalues. However, as explained above, not all solutions of the gauge-fixed equation are physical: there are "pure gauge" and "gauge-condition violating" polarizations. In harmonic gauge GR, the degeneracy of the eigenvalues can be interpreted as both types of unphysical solutions propagate at the speed of light, i.e., at the same speed as physical solutions. When we deform the theory by turning on Lovelock or Horndeski terms, the "pure gauge" and "gauge-condition violating" modes continue to propagate at the speed of light, and so these eigenvalues remain degenerate. But, generically, if eigenvalues are degenerate, then the matrix will not be diagonalizable, and this is why strong hyperbolicity fails in harmonic gauge in complicated modifications of GR.

In the absence of a well-posed formulation of the equations of motion, an alternative approach is conventional in EFT. If the coefficients of the higher-derivative terms are proportional to some small parameter ϵ, then one can seek solutions as an expansion in powers of ϵ. For example, this approach has been adopted in recent studies of EdGB theory [57, 69, 74]. This requires that the solution remains close, globally in time, to a solution of the $\epsilon = 0$ theory. However, in practice, small deviations from the $\epsilon = 0$ theory may gradually accumulate over time until they become large (e.g. this could be an orbital phase in a binary black hole spacetime). This would lead to a breakdown of the perturbative approach in a situation where the EFT equations of motion should still be valid. On the other hand, a well-posed formulation of these equations of motion would be able to accommodate such secular effects [12].

1.4 Outline

The core of this thesis is concerned with the well-posedness of the Cauchy problem in Lovelock and Horndeski theories. Chapter 2 concentrates on a simple class of Horndeski theories called cubic Horndeski theories. We will discuss three well-posed formulations of weakly coupled cubic Horndeski theories; two of these are based on extensions of methods widely used in numerical relativity, the third one is a generalization of an elliptic-hyperbolic formulation of Einstein's equation.

In chapter 3 we introduce a strongly hyperbolic formulation of general relativity, based on a modified harmonic gauge condition and gauge-fixing procedure. It is also shown, using a continuity argument, that the modified harmonic gauge equations of motion in weakly coupled Lovelock and Horndeski theories are strongly hyperbolic.

In chapter 4 we investigate the so-called initial data problem in a class of scalar-tensor effective field theories (4∂ST theories). We discuss three methods on how to construct physically interesting initial data on asymptotically flat initial hypersurfaces that satisfies the gravitational constraint equations of the EFT at weak coupling. The three methods are based on standard techniques used in mathematical and numerical general relativity.

The results are summarized in chapter 5.

1.5 Notations and conventions

Our conventions agree with those of [38] unless stated otherwise. In particular, the spacetime metric signature is chosen to be $(- + \ldots +)$. We are going to use the Latin letters $(a, b, c, ...)$ for abstract indices. Greek letters $(\mu, \nu, \rho, ...)$ stand for coordinate indices that run from 0 to $d-1$ in a d-dimensonal spacetime. The Latin letters $(i, j, k, ...)$ will be used for "spatial" indices on a $d-1$-dimensional hypersurface. For a Riemannian metric m, $|\cdot|_m$ denotes the pointwise norm with respect to m (e.g. for a vector field v^a we have $|v|_m = \sqrt{m_{ab}v^a v^b}$).

Chapter 2

Well-posed formulation of cubic Horndeski theories

In this chapter we will discuss the initial value problem for a special class of Horndeski theories, called cubic Horndeski theories. The contents of this chapter are the results of original research conducted by the author of this thesis and published in [67].

2.1 Introduction

The special class of Horndeski theories in which harmonic gauge succeeds has the property that there is no nontrivial coupling between the scalar field and the curvature of spacetime. There is, however, a more general class of Horndeski theories that is "simple" in the sense that its Lagrangian does not contain a coupling between the scalar field and the curvature but the harmonic gauge equations of motion are not strongly hyperbolic [60]. These are the theories with nontrivial $G_3(\phi, X)$ and $G_4 = G_5 = 0$, referred to as *cubic* Horndeski theories. (Note that theories with nontrivial $G_4 = G_4(\phi)$ can be reduced to theories with $G_4 = 0$ by a field redefinition.) Despite the fact that there is no coupling between the curvature and the scalar field in the cubic action, the curvature enters into the scalar equation of motion. This curvature term in the scalar equation poses the main difficulty to obtain a well-posed initial value formulation of cubic Horndeski theories.

In this chapter, we focus on cubic Horndeski theories and study its initial value formulation in more detail. We provide three formulations of this theory with strongly hyperbolic equations in the weakly coupled regime.

We begin with a general discussion of the Arnowitt-Deser-Misner (ADM) formulation of cubic Horndeski theories in Section 2.2. More specifically, we present the standard ADM evolution and constraint equations of cubic Horndeski theories and show that a suitable linear combination of these equations give a scalar evolution equation which contains no second derivatives of the spacetime metric. This observation has already been made in [75] but we emphasize this fact here again, since it is a key step to obtain well-posed formulations. The section is concluded by a preliminary discussion of constraint propagation.

In Section 2.3 we consider a version of the Baumgarte-Shapiro-Shibata-Nakamura (BSSN) formulation [76, 77] with a generalized Bona-Massó slicing condition [78] and nondynamical (i.e. arbitrary but a priori fixed) shift vector. This formulation contains a free parameter and a freely specifiable function: the function describes the slicing condition, the parameter describes how we modify the evolution system by the momentum constraint. It is shown that when the function and the parameter obey some simple bounds then the system of equations is strongly hyperbolic in the weakly coupled regime. These bounds ensure that the troublesome degeneracy between certain mode solutions (causing the failure of the original harmonic gauge in cubic Horndeski theories) is removed.

Section 2.4 focuses on the so-called covariant conformal Z4 (CCZ4) formulation [79]. The CCZ4 system was originally constructed for GR to enhance the accuracy of numerical simulations. This is achieved by an appropriate modification of Einstein's equation so that constraint violations are damped away during the evolution. We give a straightforward generalization of the CCZ4 method to cubic Horndeski theories. This involves introducing a family of dynamical gauge conditions depending on two free functions (generalized Bona-Massó slicing and "gamma driver" conditions). Strong hyperbolicity requires that these functions satisfy some simple bounds and the couplings are sufficiently small. In particular, the slicing conditions selected by strong hyperbolicity include the 1+log slicing which is used in many numerical applications. We also comment on the issue of constraint damping in cubic Horndeski theories.

Finally, in Appendix 2.A, we present an elliptic-hyperbolic formulation of cubic Horndeski theories, using ideas put forward by Andersson and Moncrief in [80] for vacuum GR. After briefly reviewing [80], we show how a suitable modification of the constant (or arbitrarily prescribed) mean curvature and the spatial harmonic gauge condition lead to second order elliptic equations for the lapse function and the shift vector. In the weakly coupled regime and on compact slices with negative Ricci curvature, existence and uniqueness of solutions to these elliptic equations are guaranteed. It is then argued that under these assumptions, the strong well-posedness result of Andersson and Moncrief for GR extends to cubic Horndeski theories.

2.2 Setting up the problem

2.2.1 Equations of motion

In this section we provide the ideas that all three formulations (presented in the subsequent sections) share.

As mentioned in the Introduction, the class of theories under consideration can be described by the action (recall $X \equiv -\frac{1}{2}(\partial\phi)^2$)

$$S = \frac{1}{16\pi G}\int \mathrm{d}^4x\sqrt{-g}\,(R + X + G_2(\phi, X) + G_3(\phi, X)\Box\phi)\,. \tag{2.1}$$

The reason for separating out X in the action is that we would like to view weakly coupled Horndeski theories as small deformations of Einstein-scalar-field theory.

Varying the action (2.1) with respect to the metric yields the equation of motion [61]

$$\begin{aligned} E_{ab} \quad \equiv \quad & G_{ab} - \frac{1}{2}\left(X + G_2 + 2X\partial_\phi G_3\right) g_{ab} - \frac{1}{2}\left(1 + \partial_X G_2 + 2\partial_\phi G_3\right)\nabla_a\phi\nabla_b\phi \\ & + \frac{1}{2}\partial_X G_3\Big(-\Box\phi\ \nabla_a\phi\nabla_b\phi + \nabla_a\phi\nabla_b\nabla_c\phi\nabla^c\phi \\ & \qquad + \nabla_b\phi\nabla_a\nabla_c\phi\nabla^c\phi - \nabla_c\nabla_d\phi\nabla^c\phi\nabla^d\phi\ g_{ab}\Big) = 0. \end{aligned} \tag{2.2}$$

In some situations, it is beneficial to use the linear combination $G_{ab} - \frac{1}{2}Gg_{ab} = R_{ab} = 0$ of the Einstein equations, rather than $G_{ab} = 0$. In fact, it turns out that it is useful to consider the same combination of the gravitational equations of motion in cubic Horndeski theories:

$$\begin{aligned} E_{ab} - \frac{1}{2}Eg_{ab} = R_{ab} & + \frac{1}{2}\left(G_2 - X\partial_X G_2 - X\partial_X G_3\Box\phi\right) g_{ab} \\ & - \frac{1}{2}\left(1 + \partial_X G_2 + 2\partial_\phi G_3\right)\nabla_a\phi\nabla_b\phi \\ & + \frac{1}{2}\partial_X G_3\left(-\Box\phi\nabla_a\phi\nabla_b\phi + 2\nabla_{(a}\phi\nabla_{b)}\nabla_c\phi\nabla^c\phi\right) = 0. \end{aligned} \tag{2.3}$$

Varying the action (2.1) with respect to ϕ gives the scalar evolution equation

$$\begin{aligned}E_\phi \equiv &-\left(1+\partial_X G_2+2X\partial_X^2 G_2+2\partial_\phi G_3+2X\partial_{X\phi}^2 G_3\right)\Box\phi\\ &-\left(\partial_X^2 G_2+2\partial_{X\phi}^2 G_3\right)\left((\partial\phi)^2\Box\phi-\nabla^a\phi\nabla^b\phi\nabla_a\nabla_b\phi\right)\\ &+\partial_X G_3 R_{ab}\nabla^a\phi\nabla^b\phi-\partial_X G_3\left((\Box\phi)^2-\nabla_a\nabla_b\phi\nabla^a\nabla^b\phi\right)\\ &+\partial_X^2 G_3\nabla^a\phi\nabla^b\phi\left(\Box\phi\nabla_a\nabla_b\phi-\nabla_a\nabla^c\phi\nabla_c\nabla_b\phi\right)\\ &+2X\left(\partial_\phi^2 G_3+\partial_{X\phi}^2 G_2\right)-\partial_\phi G_2=0.\end{aligned} \tag{2.4}$$

In this equation, the only term involving second derivatives of the metric is $R_{ab}\nabla^a\phi\nabla^b\phi$. We will see that it is useful to eliminate this term using the linear combination $\left(E_{cd}-\frac{1}{2}Eg_{cd}\right)\nabla^c\phi\nabla^d\phi$ of the gravitational equations. In other words, instead of the equation $E_\phi=0$, we are going to use

$$\begin{aligned}\tilde{E}_\phi \equiv\ & E_\phi-\partial_X G_3\left(E_{cd}-\frac{1}{2}Eg_{cd}\right)\nabla^c\phi\nabla^d\phi\\ =\ &-\left(1+\partial_X G_2+2X\partial_X^2 G_2+2\partial_\phi G_3+2X\partial_{X\phi}^2 G_3\right)\Box\phi\\ &\left(\partial_X^2 G_2+2\partial_{X\phi}^2 G_3\right)\left((\partial\phi)^2\Box\phi-\nabla^a\phi\nabla^b\phi\nabla_a\nabla_b\phi\right)\\ &-\partial_X G_3\left((\Box\phi)^2-\nabla_a\nabla_b\phi\nabla^a\nabla^b\phi\right)\\ &+\partial_X^2 G_3\nabla^a\phi\nabla^b\phi\left(\Box\phi\nabla_a\nabla_b\phi-\nabla_a\nabla^c\phi\nabla_c\nabla_b\phi\right)\\ &+2X\left(\partial_\phi^2 G_3+\partial_{X\phi}^2 G_2\right)-\partial_\phi G_2\\ &+\partial_X G_3\Big(2X^2+XG_2+X^2\partial_X G_2+X^2\partial_X G_3\Box\phi\\ &+4X^2\partial_\phi G_3+2X\partial_X G_3\nabla^a\phi\nabla^b\phi\nabla_a\nabla_b\phi\Big)=0\end{aligned} \tag{2.5}$$

as the scalar evolution equation. The reason for this is that this equation is only first order in derivatives of the metric and hence the principal terms in this equation are those involving second derivatives of the scalar field. (Some benefits of the use of this particular linear combination were also noticed in [75].)

Now we assume that the spacetime manifold (M,g) is globally hyperbolic $M=\mathbb{R}\times\Sigma$ and h_{ab} is the spatial metric induced on the spacelike Cauchy surfaces Σ_t. Let n^a be the future directed unit normal to Σ_t. The lapse function α and the shift vector β^a are then defined by

$$\left(\frac{\partial}{\partial t}\right)^a=\alpha n^a+\beta^a. \tag{2.6}$$

The convention on the extrinsic curvature used here is

$$K_{ab} = -\frac{1}{2}\mathcal{L}_n h_{ab} = -\frac{1}{2\alpha}\left(\partial_t - \mathcal{L}_\beta\right) h_{ab}. \tag{2.7}$$

We also need ADM variables for the derivatives of the scalar field: let

$$K_\phi \equiv -\frac{1}{2}\mathcal{L}_n \phi = -\frac{1}{2\alpha}\left(\partial_t - \mathcal{L}_\beta\right) \phi \tag{2.8}$$

and let D denote the covariant derivative associated with the Levi-Civita connection of h. For convenience, we also introduce a fixed, smooth background metric $\mathring{h}$ on the spatial slices and denote the corresponding covariant derivative and Christoffel symbol by $\mathring{D}$ and $\mathring{\Gamma}^i_{jk}$, respectively.

Now we are ready to provide the standard ADM-type equations of motion in cubic Horndeski theories. Taking the spatial projection of (2.3) in both indices yields the tensor evolution equation

$$\begin{aligned} 0 \; = \; & -\left(\partial_t - \mathcal{L}_\beta\right) K_{ij} - \partial_X G_3 (X h_{ij} + D_i\phi D_j\phi)\left(\partial_t - \mathcal{L}_\beta\right) K_\phi - D_i D_j \alpha \\ & + \alpha \Bigg\{ R[D]_{ij} + K K_{ij} - 2K_{ik}K^k_j - \frac{1}{2}\left(1 + \partial_X G_2 + 2\partial_\phi G_3\right) D_i\phi D_j\phi \\ & \quad + \frac{1}{2} h_{ij}\left(G_2 - X\partial_X G_2 - X\partial_X G_3\left(D^k D_k\phi - 2K_\phi K + D^k\phi D_k \ln\alpha\right)\right) \\ & \quad + \frac{1}{2}\partial_X G_3\Big(D^k\phi D_k\left(D_i\phi D_j\phi\right) - D_i\phi D_j\phi D^k D_k\phi + 2 D_i\phi D_j\phi K_\phi K \\ & \quad - D_i\phi D_j\phi D^k\phi D_k \ln\alpha - 8K_\phi D_{(i}\phi D_{j)} K_\phi\Big)\Bigg\}. \end{aligned} \tag{2.9}$$

Note that

$$X = \frac{1}{2}\left(4K_\phi^2 - D^k\phi D_k\phi\right). \tag{2.10}$$

Similarly to general relativity, the projections $E_{ab}n^a n^b$ and $E_{cb}h^c_a n^b$ in Horndeski theories yield constraint equations: the Hamiltonian constraint is

$$\begin{aligned} 2\mathbf{H} \equiv 2E_{\mu\nu}n^\mu n^\nu \; = \; & R[D] + K^2 - K_{ij}K^{ij} - \frac{1}{2}\left(D_i\phi D^i\phi + 4K_\phi^2\right) \\ & + G_2 - 4K_\phi^2 \partial_X G_2 - (4K_\phi^2 + D_i\phi D^i\phi)\partial_\phi G_3 \\ & - \partial_X G_3\Big(-8K_\phi^3 K + 4K_\phi^2 D^i D_i \phi \\ & + 2K_\phi K_{ij} D^i\phi D^j\phi - D^i\phi D^j\phi D_i D_j\phi\Big) = 0, \end{aligned} \tag{2.11}$$

while the momentum constraint reads as

$$\begin{aligned}\mathbf{M}_i \equiv E_{\mu i}n^\mu \quad = \quad & D_iK - D^jK_{ij} + (1+\partial_X G_2 + 2\partial_\phi G_3)\,K_\phi D_i\phi \\ & -\frac{1}{2}\partial_X G_3\Big(4K_\phi^2 D_i\phi K - 2K_\phi D_i\phi D^k D_k\phi - K_{kl}D^k\phi\ D^l\phi D_i\phi \\ & +2K_\phi D^j\phi\ D_jD_i\phi + 2D_i\phi D^k\phi\ D_kK_\phi - 8K_\phi^2 D_iK_\phi\Big) = 0. \qquad (2.12)\end{aligned}$$

Even though we are not going to use the explicit form of the scalar evolution equation (2.5), only some of its properties, we rewrite it in terms of the ADM variables, for reference. One obtains[1]

$$\begin{aligned}E_\phi \equiv \Phi\Bigg(& 1 + \partial_X G_2 + 4K_\phi^2\partial_X^2 G_2 + 2\partial_\phi G_3 + \partial^2_{X\phi}G_3(4K_\phi^2 + D_i\phi D_j\phi h^{ij}) + 2\Phi_{ij}\partial_X G_3 h^{ij} \\ & + \tfrac{1}{4}\Big(\partial_X G_3\Big)^2\Big(48K_\phi^4 - 8D_i\phi D_j\phi K_\phi^2 h^{ij} - D_i\phi D_j\phi D_k\phi D_l\phi h^{ik}h^{jl}\Big) \\ & + \partial_X^2 G_3\Big(4K_\phi^2\Phi_{ij}h^{ij} - D_k\phi D_l\phi\Phi_{ij}h^{ik}h^{jl}\Big)\Bigg) \\ & - \partial_\phi G_2 - \Phi_{ij}h^{ij} - 2\Phi_{ij}\partial_\phi G_3 h^{ij} + \partial^2_{X\phi}G_2(4K_\phi^2 - D_i\phi D_j\phi h^{ij}) \\ & + \partial_\phi^2 G_3(4K_\phi^2 - D_i\phi D_j\phi h^{ij}) + \tfrac{1}{2}G_2\partial_X G_3(4K_\phi^2 - D_i\phi D_j\phi h^{ij}) \\ & + \partial_X^2 G_2(4D_i\phi K_\phi\Phi_j h^{ij} + D_k\phi D_l\phi\Phi_{ij}h^{ik}h^{jl}) \\ & + \partial_X G_2\Big(-\Phi_{ij}h^{ij} + \tfrac{1}{4}\partial_X G_3\Big(16K_\phi^4 - 8D_i\phi D_j\phi K_\phi^2 h^{ij} + D_i\phi D_j\phi D_k\phi D_l\phi h^{ik}h^{jl}\Big)\Big) \\ & + \partial^2_{X\phi}G_3\Big(8D_i\phi K_\phi\Phi_j h^{ij} + 4K_\phi^2\Phi_{ij}h^{ij} + 2D_k\phi D_l\phi\Phi_{ij}h^{ik}h^{jl} - D_i\phi D_j\phi\Phi_{kl}h^{ij}h^{kl}\Big) \\ & + \partial_X G_3\Big(\partial_\phi G_3\Big(16K_\phi^4 - 8D_i\phi D^i\phi K_\phi^2 + D_i\phi D_j\phi D^i\phi D^j\phi\Big) + 8K_\phi^4 - 2\Phi_i\Phi^i \\ & - 4D_i\phi D_j\phi K_\phi^2 h^{ij} + \tfrac{1}{2}D_i\phi D_j\phi D_k\phi\ D_l\phi h^{ik}h^{jl} - \Phi_{ij}\Phi_{kl}h^{ij}\ h^{kl} + \Phi_{ij}\Phi_{kl}h^{ik}\ h^{jl}\Big) \\ & + \partial_X^2 G_3\Big(-4K_\phi^2\Phi_i\Phi_j h^{ij} + 4D_i\phi K_\phi\Phi_{jl}\Phi_k\ h^{ik}h^{jl} + D_i\phi D_j\phi\Phi_k\ \Phi_l h^{ik}h^{jl} \\ & - 4D_k\phi K_\phi\Phi_{ij}\ \Phi_l h^{ik}h^{jl} - D_i\phi D^j\phi\Phi^{ik}\ \Phi_{jk} + D^i\phi D^j\phi\Phi_{ij}\ \Phi_{kl}\ h^{kl}\Big) \\ & + \tfrac{1}{4}\Big(\partial_X G_3\Big)^2\Big(-8D_i\phi - 8K_\phi^3\Phi_j h^{ij} + 16K_\phi^4\Phi_{ij}h^{ij} + 16D_k\phi D_l\phi K_\phi^2\Phi_{ij}\ h^{ik}h^{jl} \\ & - 2D_i\phi D_k\phi 4K_\phi^2\Phi_{jl}h^{ik}h^{jl} + D_i\phi D_j\phi D_k\phi D_l\phi\ \Phi_{mn}h^{ik}h^{jl}\ h^{mn} \\ & - 4D_i\phi D_k\phi D_l\phi\ h^{ik}h^{jl}\Big(+4K_\phi\Phi_j + \ D_m\phi\Phi_{jn}h^{mn}\Big)\Big) = 0. \qquad (2.13)\end{aligned}$$

[1]The *Mathematica* package *xAct* [81] was of great help in the derivation of the equations.

where we used the following auxiliary variables

$$\Phi \equiv -\frac{2}{\alpha}\left(\partial_t - \mathcal{L}_\beta\right) K_\phi - D^i\phi D_i \ln\alpha, \tag{2.14}$$

$$\Phi_i \equiv -2D_i K_\phi + K_{ij} D^j \phi, \tag{2.15}$$

$$\Phi_{ij} \equiv D_i D_j \phi - 2K_\phi K_{ij}. \tag{2.16}$$

In the subsequent sections, we will manipulate the ADM-type equations of cubic Horndeski theory and complement them with suitable gauge conditions to obtain a system of PDEs of the form (1.75)-(1.76). Once we have such a system, we can establish the local well-posedness of the initial value problem by following the 3 steps outlined in section 1.3. In particular, strong hyperbolicity of the system can be shown by using the methods of section 1.2.5.

The different methods to write the equations in a strongly hyperbolic form will involve different sets of dynamical fields. Hence, the values of n, m and the fields u and v (introduced in section 1.2.5) will be given explicitly later on a case-by-case basis. Here, we only make a simple observation about the characteristic equation

$$\xi_0 \mathbb{A} U = \mathbb{L}(\xi_k) U \tag{2.17}$$

in cubic Horndeski theories (see section 1.2.5 for notations). It is useful to rearrange the rows of this equation so that the components corresponding to the gravitational and scalar degrees of freedom are separated: we will write $U = (U_g, U_\phi)^T$ where U_g is a $n+m-2$-component vector that corresponds to the gravitational variables (e.g. h_{ij} and K_{ij}); U_ϕ is a 2-component vector corresponding to the scalar variables ϕ and K_ϕ. Since the equations (2.8) and (2.13) contain no principal terms associated with the spacetime metric g, the matrices $\mathbb{A}$ and $\mathbb{L}(\xi_i)$ have the upper triangular form

$$\mathbb{A}(u, Du, v, D^2u, Dv) = \begin{pmatrix} \mathbb{A}_{gg}(u, Du, v) & \mathbb{A}_{g\phi}(u, Du, v) \\ 0 & \mathbb{A}_{\phi\phi}(u, Du, v, D^2u, Dv) \end{pmatrix} \tag{2.18}$$

$$\mathbb{L}(u, Du, v, D^2u, Dv) = \begin{pmatrix} \mathbb{L}_{gg}(u, Du, v) & \mathbb{L}_{g\phi}(u, Du, v) \\ 0 & \mathbb{L}_{\phi\phi}(u, Du, v, D^2u, Dv). \end{pmatrix} \tag{2.19}$$

The matrix blocks labelled by subscripts gg, $g\phi$ and $\phi\phi$ have sizes $(n+m-2)\times(n+m-2)$, $2\times(n+m-2)$ and 2×2, respectively. It is worth emphasizing that in the case of cubic Horndeski theories, the matrices $\mathbb{A}_{gg}$, $\mathbb{A}_{g\phi}$, $\mathbb{L}_{gg}$, $\mathbb{L}_{g\phi}$ depend only on the fields u,

Du and v, i.e., the gravitational evolution equations are quasilinear (see e.g. equation (2.9)).

It will be useful (especially in Section 2.4) to separate the Einstein-scalar-field theory and the Horndeski (i.e. G_2 and G_3-dependent) parts in $\mathbb{A}$ and $\mathbb{L}$:

$$\begin{aligned}\mathbb{A} &= \mathbb{A}_0 + \delta\mathbb{A},\\ \mathbb{L} &= \mathbb{L}_0 + \delta\mathbb{L}\end{aligned} \tag{2.20}$$

where $\mathbb{L}_0$ and $\mathbb{M}_0$ are associated with Einstein-scalar-field theory, $\delta\mathbb{A}$ and $\delta\mathbb{L}$ are the Horndeski corrections. The specific forms of these terms will also be given on a case-by-case basis.

Let us consider in more detail the characteristic equation corresponding to (2.5) (or (2.13)). This is obtained by selecting the second derivatives of ϕ in the linearized version of (2.5) (recall that there are no second derivatives of g in (2.5)) and substituting the derivatives by a general covector ξ_μ $\partial_\mu \to \xi_\mu \equiv (\xi_0, \xi_i)$. The result is

$$\left(P'_{\phi\phi}\right)^{\mu\nu}\xi_\mu\xi_\nu \equiv P_{\phi\phi}(\xi) - \partial_X G_3\left(P^{\mu\nu}_{g\phi}(\xi) - \frac{1}{2}g_{\rho\sigma}g^{\mu\nu}P^{\rho\sigma}_{g\phi}(\xi)\right)\nabla_\mu\phi\nabla_\nu\phi = 0 \tag{2.21}$$

where $P^{\mu\nu}_{g\phi}(\xi)$ and $P^{\mu\nu}_{\phi\phi}(\xi)$ are given by

$$P^{\mu\nu}_{g\phi}(\xi) = \frac{1}{2}\partial_X G_3\nabla^\mu\phi\nabla^\nu\phi|\xi|^2_g - \partial_X G_3\xi^\sigma\nabla_\sigma\phi\left(\xi^{(\mu}\nabla^{\nu)}\phi - \frac{1}{2}g^{\mu\nu}\xi^\rho\nabla_\rho\phi\right) \tag{2.22}$$

and

$$\begin{aligned}P_{\phi\phi}(\xi) =& \Big(1 + \partial_X G_2 + 2X\partial^2_X G_2 + 2\partial_\phi G_3 + 2X\partial^2_{X\phi}G_3\Big)|\xi|^2_g\\ &+ \left(\partial^2_X G_2 + 2\partial^2_{X\phi}G_3\right)\left((\partial\phi)^2|\xi|^2_g - (\xi_\mu\nabla^\mu\phi)^2\right)\\ &+ 2\partial_X G_3\left((\Box\phi)|\xi|^2_g - \xi^\mu\xi^\nu\nabla_\mu\nabla_\nu\phi\right)\\ &- \partial^2_X G_3\nabla^\mu\phi\nabla^\nu\phi\Big(\Box\phi\ \xi_\mu\xi_\nu + |\xi|^2_g\nabla_\mu\nabla_\nu\phi - 2\xi_\rho\xi_{(\mu}\nabla_{\nu)}\nabla^\rho\phi\Big).\end{aligned} \tag{2.23}$$

The notations $P_{g\phi}$, $P_{\phi\phi}$ and $P'_{\phi\phi}$ refer to the coefficients of the second derivatives of ϕ in the linearized versions of equations (2.2), (2.4) and (2.5), respectively. The same characteristic equation corresponding to the scalar degree of freedom has been previously found in [60] and [75].[2]

[2] More precisely, to make a comparison with [60], we note that with the preferred gauge choice $\mathcal{H}_{ab} = -\partial_X G_3\nabla_a\phi\nabla_b\phi$ (and $G_4 = 0$) made therein, equation (230) of [60] agrees with (2.21).

In the weakly coupled regime, $P'_{\phi\phi}$ is close to the spacetime metric g and therefore, it is a Lorentzian metric. This regime is defined by the criterion that Horndeski terms are small compared to the Einstein-scalar-field terms. More precisely, let $E = \max\left\{|R_{\mu\nu\rho\sigma}|^{1/2}, |\nabla_\mu\phi|, |\nabla_\mu\nabla_\nu\phi|^{1/2}\right\}$ in all orthonormal bases. Then the small coupling condition is equivalent to

$$\begin{aligned} &|\partial_X^k\partial_\phi^l G_2|E^{2k+2} \ll 1 && k = 0,1,2;\ l = 0,1; \\ &|\partial_X^k\partial_\phi^l G_3|E^{2k} \ll 1 && k, l = 0,1,2. \end{aligned} \tag{2.24}$$

Note that this condition can be satisfied when spacetime is strongly curved according to standard terminology but the function G_3 contains small enough coupling constants.

Regarding (2.21) as an equation for the "characteristic speeds" ξ_0 for given $\xi_i \neq 0$, this equation has two distinct real and nonzero solutions $\xi_0^{\phi,\pm}$. Furthermore, the weakly coupled assumptions (2.24) also ensure that the spacelike $t =$ constant hypersurfaces are noncharacteristic.

2.2.2 Constraint propagation

In addition to studying the hyperbolicity of the equations of motion in different formulations, we need to address the issue of constraint propagation (see section 1.3). That is to say, we need to check whether solutions to the equations used in these formulations remain solutions of the original Horndeski equations of motion during the evolution. Here we present a fairly detailed derivation of the equations governing the propagation of gauge conditions and constraints, even though the individual steps are quite standard. The purpose of this is to demonstrate that the Bianchi identity (and its generalization) leads straightforwardly to a homogeneous system of PDEs for the constraint variables, without making any reference to a specific form of the equations of motion. The only assumption we make is that the equations of motion are second order PDEs obtained by varying a diffeomorphism invariant action. This guarantees that the normal projection of the equations of motion is a constraint equation (i.e. an equation that does not involve second time derivatives). Note that in this section we derive the equations without gauge fixing, the effect of the gauge fixing terms on the constraint propagation system will be discussed later.

Let $E_{ab} = 0$ be the equations of motion obtained by varying the action with respect to the spacetime metric g_{ab}. Let us decompose it as

$$E_{ab} = \mathbf{E}_{ab} - n_a \mathbf{M}_b - n_b \mathbf{M}_a + n_a n_b \mathbf{H} \tag{2.25}$$

with

$$\mathbf{E}_{ab} = E_{cd} h^c_a h^d_b, \tag{2.26a}$$

$$\mathbf{H} = E_{ab} n^a n^b \tag{2.26b}$$

$$\mathbf{M}_a = E_{cb} h^c_a n^b. \tag{2.26c}$$

These variables denote the spatial evolution equation, the Hamiltonian constraint and the momentum constraint, respectively. First, we consider

$$\begin{aligned} n^b \nabla^a E_{ab} =& - \mathbf{E}_{ab} \nabla^a n^b - n^b n_a \nabla^a \mathbf{M}_b \\ &+ \nabla^a \mathbf{M}_a - n_a \nabla^a \mathbf{H} + K\mathbf{H}, \end{aligned} \tag{2.27}$$

where we used $\mathbf{E}_{ab} n^b = 0$, $\mathbf{M}_a n^a = 0$, $n_a n^a = -1$ and $\nabla^a n_a = -K$. Furthermore, the following identities hold:

$$\nabla^a \mathbf{M}_a = D^a \mathbf{M}_a + \mathbf{M}_b n^a \nabla_a n^b \tag{2.28a}$$

$$\mathbf{E}_{ab} \nabla^a n^b = -\mathbf{E}_{ab} K^{ab} \tag{2.28b}$$

$$n^b n_a \nabla^a \mathbf{M}_b = -\mathbf{M}_b n_a \nabla^a n^b = -\mathbf{M}_b \frac{D^b \alpha}{\alpha} \tag{2.28c}$$

We would like to use the spatial projection of the trace reversed version of $\mathbf{E}_{ab}$ as evolution equation[3], i.e.

$$\begin{aligned} \mathcal{E}_{ab} &= h^c_a h^d_b \left(E_{cd} - \frac{1}{2} g^{ef} E_{ef} g_{cd} \right) \\ &= \mathbf{E}_{ab} - \frac{1}{2} \mathbf{E} h_{ab} + \frac{1}{2} \mathbf{H} h_{ab}. \end{aligned}$$

Hence, we set

$$\mathbf{E}_{ab} = \mathcal{E}_{ab} + \mathbf{H} h_{ab} - \mathcal{E} h_{ab}. \tag{2.29}$$

[3]The reason why we prefer to use $\mathcal{E}_{ab} = 0$ as evolution equation rather than $\mathbf{E}_{ab} = 0$ is that in general relativity the latter approach yields only a weakly hyperbolic system of equations for the constraint variables [42].

With these identities we have

$$n^b\nabla^a E_{ab} = -\left(\partial_t - \mathcal{L}_\beta\right)\mathbf{H} + 2\alpha K\mathbf{H} + \frac{1}{\alpha}D^i\left(\alpha^2\mathbf{M}_i\right) \\ + \alpha\mathcal{E}_{ij}\left(K^{ij} - Kh^{ij}\right). \tag{2.30}$$

Next, we consider the spatial projection of the Bianchi identity

$$h^b_c\nabla^a E_{ab} = h^b_c\nabla^a\mathbf{E}_{ab} - \nabla^a n_a\mathbf{M}_c - n_a h^b_c\nabla^a\mathbf{M}_b \\ - \nabla_a n_b h^b_c\mathbf{M}_a + \mathbf{H}h^b_c n_a\nabla^a n_b. \tag{2.31}$$

In this case we use

$$h^b_c\nabla^a\mathbf{E}_{ab} = D^a\mathbf{E}_{ac} + \mathbf{E}_{ac}n^b\nabla_b n^a \tag{2.32a}$$

$$n_a h^b_c\nabla^a\mathbf{M}_b = h^b_c\left(\mathcal{L}_n\mathbf{M}_b - \mathbf{M}_a\nabla_b n^a\right) \tag{2.32b}$$

$$h^b_c\mathbf{M}_a\nabla^a n_b = h^b_c\mathbf{M}_a\nabla_b n^a = -\mathbf{M}_a K^a_b \tag{2.32c}$$

$$\mathbf{H}h^b_c n_a\nabla^a n_b = \mathbf{H}n_a\nabla^a n_c \tag{2.32d}$$

to obtain

$$\nabla^\mu E_{\mu i} = -\left(\partial_t - \mathcal{L}_\beta\right)\mathbf{M}_i + \alpha K\mathbf{M}_i + \frac{1}{\alpha}D_i\left(\alpha^2\mathbf{H}\right) \\ + D^j\left[\alpha\left(\mathcal{E}_{ij} - \mathcal{E}h_{ij}\right)\right] \tag{2.33}$$

(cf. eqn. (103,104) in [42]).

Now we consider the generalized version of the Bianchi identity, that is,

$$\nabla^a E_{ab} - E_\phi\nabla_b\phi = 0 \tag{2.34}$$

which is a consequence of the diffeomorphism invariance of the Horndeski action. Recall that we wish to use $\tilde{E}_\phi = 0$ as the scalar evolution equation. For this reason we set

$$E_\phi = \tilde{E}_\phi + \partial_X G_3\left(E_{cd} - \frac{1}{2}Eg_{cd}\right)\nabla^c\phi\nabla^d\phi. \tag{2.35}$$

Putting together equations (2.30), (2.33), (2.34) and (2.35) gives the equations governing the evolution of the momentum and Hamiltonian constraints

$$\begin{aligned}(\partial_t - \mathcal{L}_\beta)\,\mathbf{H} = {} & 2\alpha K\mathbf{H} + \frac{1}{\alpha}D^i\left(\alpha^2\mathbf{M}_i\right) + \alpha\mathcal{E}_{ij}\left(K^{ij} - Kh^{ij}\right) + 2\tilde{E}_\phi K_\phi \\ & + 2\alpha\partial_X G_3 K_\phi\left(\mathcal{E}_{ij}D^i\phi D^j\phi + 2\mathbf{H}4K_\phi^2 + 4\mathcal{E}K_\phi^2 + 4K_\phi\mathbf{M}_i D^i\phi\right)\end{aligned} \tag{2.36}$$

$$\begin{aligned}(\partial_t - \mathcal{L}_\beta)\,\mathbf{M}_i = {} & \alpha K\mathbf{M}_i + \frac{1}{\alpha}D^i\left(\alpha^2\mathbf{H}\right) + D^j\left[\alpha\left(\mathcal{E}_{ij} - \mathcal{E}h_{ij}\right)\right] - \tilde{E}_\phi D_i\phi \\ & - \alpha\partial_X G_3 D_i\phi\left(\mathcal{E}_{ij}D^i\phi D^j\phi + 2\mathbf{H}4K_\phi^2 + 4\mathcal{E}K_\phi^2 + 4K_\phi\mathbf{M}_i D^i\phi\right).\end{aligned} \tag{2.37}$$

In both of these equations, the terms in the second line arise due to the fact that we use equation (2.13) instead of (2.4) as the scalar equation of motion. Note that in each of the formulations studied in this paper, the tensor evolution equation is modified with gauge fixing terms. In other words, the equation $\mathcal{E}_{ij} = 0$ is replaced with a different equation which introduces additional terms into equations (2.36)-(2.37). This will be analysed on a case-by-case basis.

2.3 BSSN formulation

2.3.1 Equations of motion

The Baumgarte-Shapiro-Shibata-Nakamura (BSSN) formulation is widely used in numerical relativity. Several versions of this approach give rise to a strongly hyperbolic form of the Einstein equations [43, 82, 83]. Here, we extend this approach to cubic Horndeski theories.

The starting point to obtain the BSSN equations of motion is the standard ADM decomposition discussed in Section 2.2. We introduce the conformal metric $\tilde{h}_{ij}$ as a new variable, defined by

$$\tilde{h}_{ij} \equiv e^{-4\Omega}h_{ij} \tag{2.38}$$

where the conformal factor Ω is

$$\Omega \equiv \frac{1}{12}\ln\frac{h}{\mathring{h}} \tag{2.39}$$

for an arbitrary smooth background metric $\mathring{h}_{ij}$. Note that this implies that $\det\mathring{h} = \det\tilde{h}$. The inverse conformal metric, denoted by $\tilde{h}^{ij}$ is then

$$\tilde{h}^{ij} = e^{4\Omega}h^{ij}. \tag{2.40}$$

Next, we define the quantity[4]

$$\tilde{V}^i \equiv \tilde{h}^{kl}\left(\tilde{\Gamma}^i_{kl} - \mathring{\Gamma}^i_{kl}\right) = -\mathring{D}_j \tilde{h}^{ij} \tag{2.41}$$

where $\mathring{\Gamma}$ and $\mathring{D}$ denote the Christoffel symbol and the covariant derivative corresponding to $\mathring{h}_{ij}$. Similarly, let $\tilde{D}$ be the covariant derivative corresponding to the metric $\tilde{h}$ and let us adapt the convention that the index of $\tilde{D}_i\phi$ is raised with $\tilde{h}$ (although, clearly, the definition of $\tilde{D}_i\phi$ does not depend on $\tilde{h}$), i.e.

$$\tilde{D}^i\phi \equiv \tilde{h}^{ij}\tilde{D}_j\phi. \tag{2.42}$$

We emphasize, however, that the index of $D_i\phi$ is raised using h. We continue to use a similar convention in the further discussion: indices of tensor fields whose notation involves a tilde are raised and lowered with $\tilde{h}$, whereas indices of tensor fields without a tilde are raised and lowered with h.

The extrinsic curvature is decomposed to its trace and conformal traceless parts

$$K_{ij} \equiv e^{4\Omega}\left(\tilde{A}_{ij} + \frac{1}{3}\tilde{h}_{ij}K\right), \tag{2.43}$$

or alternatively,

$$\tilde{A}_{ij} \equiv e^{-4\Omega}\left(K_{ij} - \frac{1}{3}h_{ij}K\right). \tag{2.44}$$

The evolution equations for the variables $\tilde{h}_{ij}$ and Ω can be straightforwardly obtained using the equations (2.7), (2.38) and (2.39) (see e.g. [84] for more details):

$$\partial_0\tilde{h}_{ij} = -2\alpha\tilde{A}_{ij} + 2\tilde{h}_{k(i}\mathring{D}_{j)}\beta^k - \frac{2}{3}\tilde{h}_{ij}\mathring{D}_k\beta^k \tag{2.45}$$

$$\partial_0\Omega = -\frac{\alpha}{6}K + \frac{1}{6}\mathring{D}_k\beta^k \tag{2.46}$$

where ∂_0 is given by

$$\partial_0 \equiv \partial_t - \beta^k\mathring{D}_k. \tag{2.47}$$

To write the remaining equations in a more compact way, we use the conformal versions of the auxiliary variables introduced in (2.14):

[4] Note that the variable $\tilde{V}^i$ is often denoted by $\tilde{\Gamma}^i$ in other references.

$$
\begin{aligned}
\tilde{\Phi} \equiv \Phi = & \frac{1}{\alpha}\left(-2\partial_0 K_\phi - e^{-4\Omega}\tilde{h}^{ij}\tilde{D}_i\phi\tilde{D}_j\alpha\right), & (2.48)\\
\tilde{\Phi}_i \equiv \Phi_i = & -2\tilde{D}_i K_\phi + \tilde{A}_{ik}\tilde{D}_j\phi\tilde{h}^{jk} + \tfrac{1}{3}K\tilde{D}_i\phi, & (2.49)\\
\tilde{\Phi}_{ij} \equiv \Phi_{ij} = & \tilde{D}_i\tilde{D}_j\phi - 2\Big(\tilde{D}_j\phi\tilde{D}_i\Omega + \tilde{D}_i\phi\tilde{D}_j\Omega - \tilde{h}_{ij}\tilde{h}^{kl}\tilde{D}_k\phi\tilde{D}_l\Omega\Big)\\
& -2K_\phi e^{4\Omega}\Big(\tilde{A}_{ij} + \tfrac{1}{3}K\tilde{h}_{ij}\Big). & (2.50)
\end{aligned}
$$

The evolution equation for K is the trace of the tensor evolution equation, i.e. the same as (2.131), except that the variables h_{ij} and K_{ij} (and the covariant derivatives) are now replaced by the "conformal" variables introduced in (2.38)-(2.43):

$$
\begin{aligned}
0 \;=\; & -\partial_0 K - \alpha\Phi\partial_X G_3\Big(3K_\phi^2 - \tfrac{1}{4}\tilde{D}_i\phi\tilde{D}_j\phi\;\tilde{h}^{ij}e^{-4\Omega}\Big) - \tilde{h}^{ij}\tilde{D}_i\tilde{D}_j\alpha\\
& -2\tilde{h}^{ij}\tilde{D}_i\alpha\tilde{D}_j\Omega + \alpha\Big\{\tilde{A}_{ik}\tilde{A}_{jl}\tilde{h}^{ij}\tilde{h}^{kl} + \tfrac{1}{3}K^2 + 2K_\phi^2 + 4\partial_\phi G_3 K_\phi^2\\
& +\tfrac{1}{2}G_2 + \tfrac{1}{4}\partial_X G_2\Big(4K_\phi^2 + \tilde{D}_i\phi\tilde{D}_j\phi\tilde{h}^{ij}e^{-4\Omega}\Big).\\
& +\partial_X G_3 e^{-4\Omega}\Big(K_\phi^2\tilde{\Phi}_{ij}\;\tilde{h}^{ij} - \tilde{D}_i\phi A\tilde{\Phi}_j\tilde{h}^{ij} + \tfrac{1}{4}\tilde{D}_i\phi\tilde{D}_j\phi\tilde{\Phi}_{kl}\;\tilde{h}^{ij}\tilde{h}^{kl}e^{-4\Omega}\Big)\Big\} \quad (2.51)
\end{aligned}
$$

The equation describing the evolution of $\tilde{A}_{ij}$ is obtained by taking the trace free part of (2.9) and writing it in conformal variables:

$$
\begin{aligned}
0 \;=\; & -\partial_0\tilde{A}_{ij} - \frac{\alpha}{2}e^{-4\Omega}\partial_X G_3\left(\tilde{D}_i\phi\tilde{D}_j\phi - \frac{1}{3}\tilde{h}_{ij}\tilde{D}^k\phi\tilde{D}_k\phi\right)\Phi\\
& +\alpha e^{-4\Omega}\Big[R[D]_{ij} - \tfrac{1}{\alpha}\tilde{D}_i\tilde{D}_j\alpha + 4\tilde{D}_{(i}\Omega\tilde{D}_{j)}\ln\alpha - \frac{1}{2}\Big(1 + \partial_X G_2 + 2\partial_\phi G_3\Big)\tilde{D}_i\phi\tilde{D}_j\phi\\
& +\partial_X G_3\Big(2K_\phi\tilde{D}_{(i}\phi\tilde{\Phi}_{j)} - \tfrac{1}{2}\tilde{D}_i\phi\tilde{D}_j\phi\tilde{\Phi}_{kl}\tilde{h}^{kl}e^{-4\Omega} + \tilde{D}_k\phi\tilde{D}_{(i}\phi\tilde{\Phi}_{j)l}\;\tilde{h}^{kl}e^{-4\Omega}\Big)\Big]^{\mathrm{TF}}\\
& +\alpha K\tilde{A}_{ij} - 2\alpha\tilde{A}_{ik}\tilde{A}^k{}_j + 2\tilde{A}_{k(i}\mathring{D}_{j)}\beta^k - \frac{2}{3}\tilde{A}_{ij}\mathring{D}_k\beta^k \quad (2.52)
\end{aligned}
$$

where $\tilde{T}^{TF}_{ij}$ denotes the trace free part of a symmetric tensor T_{ij},

$$
\tilde{T}^{TF}_{ij} \equiv \tilde{T}_{ij} - \frac{1}{3}\tilde{T}_{kl}\tilde{h}^{kl}\tilde{h}_{ij}, \quad (2.53)
$$

and the conformal decomposition of the spatial Ricci tensor is given by

$$\begin{aligned} R[D]_{ij} = & -\frac{1}{2}\tilde{h}^{kl}\mathring{D}_k\mathring{D}_l\tilde{h}_{ij} + \tilde{h}_{k(i}\mathring{D}_{j)}\tilde{V}^k - \frac{1}{2}\tilde{V}^k\mathring{D}_k\tilde{h}_{ij} + \left(\tilde{\Gamma}^k_{il} - \mathring{\Gamma}^k_{il}\right)\left(\tilde{\Gamma}^l_{kj} - \mathring{\Gamma}^l_{kj}\right) \\ & - \mathring{D}_k\tilde{h}_{l(i}\mathring{D}_{j)}\tilde{h}^{kl} - 2\tilde{D}_i\tilde{D}_j\Omega - 2\tilde{h}_{ij}\tilde{D}^k\tilde{D}_k\Omega + 4\tilde{D}_i\Omega\tilde{D}_j\Omega - 4\tilde{h}_{ij}\tilde{D}^k\Omega\tilde{D}_k\Omega. \end{aligned} \tag{2.54}$$

We can write down an evolution equation for $\tilde{V}^i$ by taking the time derivative of (2.41) and commuting ∂_0 with $\mathring{D}$ on the RHS to get

$$\partial_0\tilde{V}^i = -2\alpha\mathring{D}_j\tilde{A}^{ij} - 2\tilde{A}^{ij}\mathring{D}_j\alpha - \tilde{V}^k\mathring{D}_k\beta^i + \frac{2}{3}\tilde{V}^i\mathring{D}_k\beta^k + \tilde{h}^{kl}\mathring{D}_k\mathring{D}_l\beta^i + \frac{1}{3}\tilde{h}^{ij}\mathring{D}_j\mathring{D}_k\beta^k. \tag{2.55}$$

It is useful to modify (2.55) by adding the momentum constraint times $2p\alpha$ to it where p is an arbitrary constant (real) parameter. The result is

$$\begin{aligned} \partial_0\tilde{V}^i \;=\; & -2\tilde{A}^{ij}\mathring{D}_j\alpha - \tilde{V}^k\mathring{D}_k\beta^i + \frac{2}{3}\tilde{V}^i\mathring{D}_k\beta^k + \tilde{h}^{kl}\mathring{D}_k\mathring{D}_l\beta^i + \frac{1}{3}\tilde{h}^{ij}\mathring{D}_j\mathring{D}_k\beta^k + \\ & \alpha\Big\{2(p-1)\tilde{D}_k\tilde{A}^{ki} - \frac{4p}{3}\tilde{D}^iK + 2p\tilde{h}^{ij}\Big[-\Big(1 + \partial_X G_2 + 2\partial_\phi G_3\Big)K_\phi\tilde{D}_j\phi \\ & -\frac{1}{2}\partial_X G_3\Big(-4K_\phi^2\tilde{\Phi}_j - 2\tilde{D}_l\phi K_\phi\tilde{\Phi}_{jk}\tilde{h}^{kl}e^{-4\Omega} \\ & +2\tilde{D}_j\phi K_\phi\tilde{\Phi}_{kl}\tilde{h}^{kl}e^{-4\Omega} + \tilde{D}_k\phi\tilde{D}_j\phi\tilde{\Phi}_l\;\tilde{h}^{kl}e^{-4\Omega}\Big)\Big]\Big\}. \end{aligned} \tag{2.56}$$

The benefit of using (2.56) rather than (2.55) will become clear later: we will show that for a range of values of the parameter p, the system is strongly hyperbolic.

Finally, once again we use $\tilde{E}_\phi = 0$ as the scalar evolution equation (defined in (2.5)) which can also be rewritten in terms of the variables introduced in this section:

$$\partial_0\phi = -2\alpha K_\phi \tag{2.57}$$

$$\begin{aligned} 2\partial_0 K_\phi \;=\; & -e^{-4\Omega}\tilde{h}^{ij}\tilde{D}_i\phi\tilde{D}_j\alpha - \alpha e^{-4\Omega}\tilde{D}_i\tilde{D}_j\phi + 2\alpha K_\phi\Big(\tilde{A}_{ij} + \tfrac{1}{3}K\tilde{h}_{ij}\Big) \\ & +2\alpha e^{-4\Omega}\Big(\tilde{D}_j\phi\tilde{D}_i\Omega + \tilde{D}_i\phi\tilde{D}_j\Omega - \tilde{h}_{ij}\tilde{h}^{kl}\tilde{D}_k\phi\tilde{D}_l\Omega\Big) \\ & +\delta\tilde{E}_\phi(\phi, \tilde{D}\phi, \tilde{D}\tilde{D}\phi, K_\phi, \tilde{D}K_\phi, \tilde{h}, \Omega, \alpha) \end{aligned} \tag{2.58}$$

where $\delta\tilde{E}_\phi$ stands for all the Horndeski correction terms in the scalar equation. It is straightforward to compute these terms explicitly from (2.13) but we will not need the explicit form of these terms.

Equations (2.45), (2.46), (2.51), (2.52), (2.56) and (2.58) must be complemented with the evolution equations for the lapse function and the shift vector. This can be done by choosing an appropriate slicing condition and a spatial coordinate condition. A popular choice for the slicing condition is harmonic slicing and its generalizations. Harmonic slicing means that the harmonic coordinate condition is imposed only on the time coordinate

$$\Box_g t = 0.$$

Writing this out in terms of the ADM variables gives an evolution equation for the lapse function:

$$\partial_0 \alpha = -\alpha^2 K. \tag{2.59}$$

Sometimes it is more convenient to consider a generalization of this condition, called the Bona-Massó slicing condition

$$\partial_0 \alpha = -\alpha^2 F(t, x, \alpha, K) \tag{2.60}$$

for a suitable function F. The choice $F(\alpha) = \frac{2}{\alpha} K$, called the 1+log slicing, is the most widely used in numerical relativity simulations. As we will see later, strong hyperbolicity of the BSSN system will enforce a condition on the function F. More precisely, the condition

$$\sigma(t, x, \alpha, K) \equiv \frac{\partial F}{\partial K}(t, x, \alpha, K). \tag{2.61}$$

There are a number of ways to impose a dynamical gauge condition on the shift vector in general relativity. However, it has also been demonstrated that it is possible to write Einstein's equations in a strongly hyperbolic form by choosing an arbitrary (but a priori fixed) shift vector [82]. This means that the shift vector only plays the role of a source term in the equations. In this section we take this approach and show that the equations of motion of cubic Horndeski theories can be written in a strongly hyperbolic form with arbitrarily fixed shift vector.

2.3.2 Proof of strong hyperbolicity

In this section, we are going to show that the BSSN equations of motion (consisting of equations (2.45), (2.46), (2.51), (2.52), (2.56), (2.60), (2.57), (2.58)) is a strongly hyperbolic system for the dynamical variables, for an appropriate choice of the parameter p and the function σ. Our strategy will be to follow the procedure outlined in section

1.2.5. Making the substitutions

$$u = (\alpha, \Omega, \tilde{h}_{ij}, \phi) \qquad \text{and} \qquad v = (K, \tilde{A}_{ij}, \tilde{V}^i, K_\phi) \tag{2.62}$$

the BSSN system has the same form as (1.75)-(1.76). In this case, we have $n = 9$ and $m = 11$.

Note that in this section our choice of basis is slightly different from the one used in Section 1.2.5: here we use $\partial_0 \equiv \partial_t - \beta^k \partial_k$, rather than $\partial_0 \equiv \partial_t$. Clearly, this only amounts to a shift in the zeroth component of a characteristic covector $\xi_0 \to \xi_0 - \beta^k \xi_k$. Nevertheless, from now on, we will denote these components by ξ_0 in the new basis. This includes the solutions $\xi_0^{\pm,\phi}$ to the scalar characteristic equation (2.21).

Next, we analyze the characteristic equation (2.17) and determine the eigenvalues ξ_0 and the corresponding eigenvectors explicitly. We will write the components of the eigenvectors U associated with the variables u as

$$t = (\hat{\alpha}, \hat{\omega}, \hat{\tilde{\gamma}}_{ij}, \hat{\phi}) \tag{2.63}$$

and the components associated with v as

$$s = (\hat{\kappa}, \hat{q}_{ij}, \hat{\tilde{v}}_i, \hat{a}) \tag{2.64}$$

in the same order as in (2.62). Now we simply write down the rows of the characteristic equations for the 20 variables listed above:

$$0 = -\xi_0 \hat{\alpha} - 2\alpha^2 \sigma \hat{\kappa} \tag{2.65a}$$

$$\begin{aligned} 0 \;=\; & -\xi_0 \hat{\kappa} - \frac{1}{2} \partial_X G_3 (12 K_\phi^2 - D_k \phi D^k \phi) \xi_0 \hat{a} \\ & + \alpha e^{-4\Omega} \Big\{ -\frac{1}{\alpha} |\xi|_{\tilde{h}}^2 \hat{\alpha} - 4 \partial_X G_3 K_\phi \tilde{D}^k \phi \; \xi_k \hat{a} \\ & \qquad + \frac{1}{4} \partial_X G_3 (4 K_\phi^2 + D^k \phi D_k \phi) |\xi|_{\tilde{h}}^2 \hat{\phi} \Big\} \end{aligned} \tag{2.65b}$$

$$0 = -\xi_0 \hat{\omega} - \frac{\alpha}{6} \hat{\kappa} \tag{2.65c}$$

$$0 = -\xi_0 \hat{\phi} - 2\alpha \hat{a} \tag{2.65d}$$

$$0 = -\xi_0 \hat{\tilde{\gamma}}_{ij} - 2\alpha \hat{\tilde{q}}_{ij} \tag{2.65e}$$

$$
\begin{aligned}
0 \;=\; & -\xi_0\hat{\tilde{q}}_{ij} - e^{-4\Omega}\partial_X G_3\left(\tilde{D}_i\phi\tilde{D}_j\phi - \frac{1}{3}\tilde{h}_{ij}\tilde{D}^k\phi\tilde{D}_k\phi\right)\xi_0\hat{a} \\
& +\alpha e^{-4\Omega}\Big\{-\frac{1}{2}|\xi|^2_{\tilde{h}}\hat{\tilde{\gamma}}_{ij} + \xi_{(i}\hat{\tilde{v}}_{j)} - \frac{1}{3}\xi_k\hat{\tilde{v}}^k\tilde{h}_{ij} \\
& \qquad -2\xi_i\xi_j\hat{\omega} + \frac{2}{3}|\xi|^2_{\tilde{h}}\hat{\omega}\tilde{h}_{ij} - \frac{1}{\alpha}\xi_i\xi_j\hat{\alpha} + \frac{1}{3}\frac{1}{\alpha}|\xi|^2_{\tilde{h}}\hat{\alpha}\tilde{h}_{ij} \\
& \qquad -4K_\phi\partial_X G_3\hat{a}\left(\tilde{D}_{(i}\phi\;\xi_{j)} - \frac{1}{3}\tilde{D}^k\phi\;\xi_k\tilde{h}_{ij}\right) \\
& \qquad -e^{-4\Omega}\partial_X G_3\hat{\phi}\bigg(\frac{1}{2}(\tilde{D}_i\phi\tilde{D}_j\phi - \frac{1}{3}\tilde{h}_{ij}\tilde{D}^k\phi\tilde{D}_k\phi)|\xi|^2_{\tilde{h}} \\
& \qquad -\tilde{D}^k\phi\tilde{D}_{(i}\phi\xi_{j)}\xi_k + \frac{1}{3}\tilde{D}^k\phi\tilde{D}^l\phi\xi_k\xi_l\tilde{h}_{ij}\bigg)\Big\}
\end{aligned}
\tag{2.65f}
$$

$$
\begin{aligned}
0 \;=\; & -\xi_0\hat{\tilde{v}}^i + \alpha\bigg(2(p-1)\xi_k\hat{\tilde{q}}^{ki} - \frac{4p}{3}\xi^i\hat{\kappa} - 8p\partial_X G_3 K_\phi^2\;\xi^i\hat{a} \\
& +2e^{-4\Omega}p\partial_X G_3\left(K_\phi\tilde{D}^k\phi\xi_k\xi^i\hat{\phi} + K_\phi\tilde{D}^i\phi|\xi|^2_{\tilde{h}}\hat{\phi} - \tilde{D}^i\phi\tilde{D}^k\phi\;\xi_k\hat{a}\right)\bigg).
\end{aligned}
\tag{2.65g}
$$

$$
0 = -\xi_0\mathcal{A}\hat{a} + \mathcal{B}(\xi_i)\hat{a} + \mathcal{C}(\xi_i)\hat{\phi} \tag{2.65h}
$$

where the coefficients $\mathcal{A}$, $\mathcal{B}$, $\mathcal{C}$ depend on the background fields and ξ_i, and their explicit form is not important for our purposes (although it is straightforward to obtain them from (2.58)). The only thing we need to know about these coefficients is that (2.155b) into (2.155d) gives

$$
\hat{\phi}\left(P'_{\phi\phi}\right)^{\mu\nu}\xi_\mu\xi_\nu = 0, \tag{2.66}
$$

i.e., equation (2.21).

Now we list the characteristic eigenvalues and the corresponding polarization of the system (2.65). It is convenient to rescale the variable ξ_0 by introducing

$$
\bar{\xi}_0 \equiv \frac{\xi_0}{\alpha e^{-2\Omega}|\xi|_{\tilde{h}}} = \frac{\xi_0}{\alpha|\xi|_h}. \tag{2.67}
$$

Due to the lower triangular structure of the characteristic equation (see section 2.2), there exists a subset of eigenvalues and eigenvectors of (2.65) with $\hat{\phi} = \hat{a} = 0$. These 18 eigenvalues and eigenvectors are the same as in the case of vacuum GR (c.f. section IV of [82]).

	$\hat{\alpha}$	$\hat{\omega}$	$\hat{\kappa}$	$\hat{\bar{\gamma}}_{ij}$	$\hat{\bar{v}}_i$	$\bar{\xi}_0$
I.	0	0	0	$\tilde{\gamma}^{TT}_{ij}$	0	± 1
II.	0	0	0	$\tilde{h}_{ij} - \frac{\xi_i\xi_j}{\lvert\xi\rvert^2_{\tilde{h}}}$	0	± 1
III.	0	0	0	$\xi_{(i}e_{j)}$	$-\frac{p-1}{2}\lvert\xi\rvert^2_{\tilde{h}} e_i$	$\pm\sqrt{p}$
IV.	0	$\hat{\omega}$	0	$\frac{2}{\lvert\xi\rvert^2_{\tilde{h}}}\left(\xi_{(i}\hat{\bar{v}}_{j)} - 2\xi_i\xi_j\hat{\omega}\right)^{\mathrm{TF}}$	$\hat{\bar{v}}_i$	0
V.	$\alpha\sigma$	$\frac{1}{12}$	$\mp\frac{\sqrt{2\sigma}}{2\alpha}$	$\left(\frac{\xi_i\xi_j}{\lvert\xi\rvert^2_{\tilde{h}}}\right)^{\mathrm{TF}}$	$\frac{2}{3}\xi_i$	$\pm\sqrt{2\sigma}$
VI.	0	0	0	$\left(\frac{\xi_i\xi_j}{\lvert\xi\rvert^2_{\tilde{h}}}\right)^{\mathrm{TF}}$	$2(p-1)\xi_i$	$\pm\sqrt{\frac{4p-1}{3}}$

Table 2.1 The list of eigenvalues and eigenvectors of the principal symbol with $\hat{\phi} = \hat{a} = 0$.

I. Transverse-traceless (physical) modes, satisfying

$$\xi^i\hat{\bar{\gamma}}^{TT}_{ij} = 0, \qquad \text{and} \qquad \tilde{h}^{ij}\hat{\bar{\gamma}}^{TT}_{ij} = 0. \tag{2.68}$$

The corresponding characteristic covectors are null, i.e. $\bar{\xi}_0 = \pm 1$. The two sign choices correspond to "ingoing" and "outgoing" mode solutions. Since there are two linearly independent transverse-traceless symmetric tensors $\hat{\bar{\gamma}}^{TT}_{ij}$, the eigenvectors span a 2-dimensional space for both sign choices (this is 4 independent eigenvectors overall).

II. Transverse but not traceless (in the sense of (2.68)) modes with null characteristics (i.e. $\bar{\xi}_0 = \pm 1$). This gives only a 1-dimensional space for both sign choices (2 independent eigenvectors overall). These modes are "constraint-violating" since the $\hat{\bar{q}}_{ij}$ components are not traceless.

III. Modes with $\hat{\bar{\gamma}}_{ij} = \xi_{(i}e_{j)}$ for any e_i orthogonal to ξ_i w.r.t. $\tilde{h}_{ij}$ and $\bar{\xi}_0 = \pm\sqrt{p}$. These modes span a 2-dimensional eigenspace for both signs (4 independent polarizations in total).

IV. Zero speed modes ($\bar{\xi}_0 = 0$) with

$$\hat{\tilde{\gamma}}_{ij} = \frac{2}{|\xi|^2_{\tilde{h}}} \left(\xi_{(i} \hat{\tilde{v}}_{j)} - 2\xi_i \xi_j \hat{\omega} \right)^{\mathrm{TF}} \tag{2.69}$$

where $\hat{\omega}$ and $\hat{\tilde{v}}_i$ are arbitrary, spanning a 4-dimensional degenerate eigenspace. To see the interpretation of these mode solutions, consider the high frequency limit of an infinitesimal diffeomorphism generated by a vector field Y orthogonal to ∂_0. This gauge transformation changes only the ij components of the metric:

$$\delta h_{ij} = \xi_{(i} Y_{j)}. \tag{2.70}$$

We can also write the change in h_{ij} in terms of the conformal variables:

$$\delta h_{ij} = \delta \left(e^{4\Omega} \tilde{h}_{ij} \right) = 4\tilde{h}_{ij} e^{4\Omega} \delta\Omega + e^{4\Omega} \delta \tilde{h}_{ij}. \tag{2.71}$$

Hence, the change in the conformal metric induced by this transformation is

$$\delta \tilde{h}_{ij} = e^{-4\Omega} \xi_{(i} Y_{j)} - 4\tilde{h}_{ij} \delta\Omega. \tag{2.72}$$

Now notice that with the choice

$$\hat{\omega} = \delta\Omega, \qquad \hat{\tilde{v}}_i = \frac{1}{2} e^{-4\Omega} |\xi|^2_{\tilde{h}} Y_i - \frac{1}{2} \left(e^{-4\Omega} \xi^i Y_i - 8\delta\Omega \right) \xi_i \tag{2.73}$$

we have

$$\begin{aligned} \hat{\tilde{\gamma}}_{ij} &= \frac{2}{|\xi|^2_{\tilde{h}}} \left(\xi_{(i} \hat{\tilde{v}}_{j)} - 2\xi_i \xi_j \hat{\omega} \right)^{\mathrm{TF}} = \delta \tilde{h}_{ij}, && (2.74) \\ \hat{\tilde{v}}^i &= -\xi_j \delta \tilde{h}^{ij} = \xi^j \tilde{h}^{ik} \delta \tilde{h}_{jk}. && (2.75) \end{aligned}$$

Therefore, we can interpret the 3 independent choices of zero speed modes, corresponding to 3 linearly independent choices of Y_i in (2.73) as pure gauge modes associated with spatial diffeomorphisms. The remaining zero speed eigenmode can be obtained by setting e.g. $\hat{\omega} \neq 0$ and $\hat{\tilde{v}}_i = 0$. This mode violates the high-frequency version of the constraint equation (2.41), since $\xi^i \hat{\tilde{\gamma}}_{ij} \neq \hat{\tilde{v}}_j$.

V. A 1-dimensional space of modes with $\bar{\xi}_0 = \pm\sqrt{2\sigma}$, for both sign choices. An argument similar to IV. establishes that these modes are also pure gauge, corresponding to an infinitesimal change of the slicing in the high-frequency limit.

VI. A two-dimensional space of modes with $\bar{\xi}_0 = \pm\sqrt{\frac{4p-1}{3}}$. These modes also violate the high-frequency version of (2.41), since $\xi^i \hat{\tilde{\gamma}}_{ij} \neq \hat{\tilde{v}}_j$.

The expressions for the eigenvectors are listed in Table 2.1. It is clear that the eigenvalues are real and the eigenvectors are smooth functions of their arguments when $\sigma > 0$ and $p > \frac{1}{4}$.

For strong hyperbolicity, we need 20 linearly independent eigenvectors with real eigenvalues and smooth dependence on ξ_i. Since we have already found 18, it remains to find two additional eigenvalues and eigenvectors with nontrivial $\hat{\phi}$ and $\hat{a}$. The eigenvalues corresponding to these eigenvectors are found by solving the system consisting of equations (2.65d) and (2.65h), or equivalently, (2.21). As mentioned before, this equation has two distinct real solutions $\xi_0^{\phi,\pm}$ when the Horndeski terms are much smaller than the Einstein-scalar-field terms (see the end of Section 2.2 and equation (2.24)). Therefore, at weak coupling, there must indeed be 2 additional eigenvectors. The only thing that needs to be shown is the condition on smooth dependence.

A nice way to obtain the corresponding eigenvectors is to derive a closed equation containing $\hat{\phi}$ and the variables

$$\hat{a}^\phi \equiv -\tfrac{1}{2\alpha}\xi_0^{\phi,\pm}\hat{\phi}, \qquad \text{and} \qquad \hat{\kappa}_{ij} = e^{4\Omega}\hat{\tilde{q}}_{ij} + \frac{1}{3}\hat{\kappa}h_{ij}. \tag{2.76}$$

Equations (2.65) imply

$$\begin{aligned} 0 \;=\; & -|\xi^{\phi,\pm}|_g^2\Big(\hat{\kappa}_{ij} + \partial_X G_3(X h_{ij} + D_i\phi D_j\phi)\hat{a}^\phi - 2\partial_X G_3 K_\phi D_{(i}\phi\;\xi_{j)}\hat{\phi}\Big) \\ & +(2p-2\sigma-1)\xi_i\xi_j\hat{\kappa} - 2(p-1)\xi_{(i}\hat{\kappa}_{j)\xi} - \frac{2}{3}(p-1)(|\xi|_h^2\hat{\kappa} - \hat{\kappa}_{\xi\xi})h_{ij} \\ & +\partial_X G_3\Big\{(p-1)D_{(i}\phi\;\xi_{j)}\left(-2D^k\phi\;\xi_k\hat{a}^\phi + 2K_\phi|\xi|_h^2\hat{\phi}\right) \\ & +\xi_i\xi_j\left(8pK_\phi^2\hat{a}^\phi - 2pK_\phi D^k\phi\;\xi_k\hat{\phi}\right) - \frac{2}{3}(p-1)\hat{a}^\phi\left(4K_\phi^2|\xi|_h^2 - (D^k\phi\;\xi_k)^2\right)h_{ij}\Big\} \end{aligned} \tag{2.77}$$

where we introduced $\hat{\kappa}_{i\xi} \equiv \hat{\kappa}_{ij}\xi^j$ and

$$|\xi^{\phi,\pm}|_g^2 = -(\xi_0^{\phi,\pm})^2 + \alpha^2|\xi|_h^2.$$

Note that in (2.77) we raise and lower indices with the metric h.

It is easy to see that if the solutions $\hat{\kappa}_{ij}^{\phi,\pm}$ of (2.77) are smooth functions of ξ_i, then one can solve (2.76) and (2.65) for the variables $\hat{\tilde{q}}_{ij}$, $\hat{\kappa}$, $\hat{\tilde{\gamma}}_{ij}$, $\hat{\tilde{v}}_i$, $\hat{\omega}$ and $\hat{\alpha}$. Based on the tensorial structure of (2.77), we can look for an eigenvector of the form

$$\hat{\kappa}^{\phi}_{ij} = c_1\xi_i\xi_j + c_2|\xi|^2_h h_{ij} + c_3 D_i\phi D_j\phi + 2c_4 D_{(i}\phi\, \xi_{j)}. \tag{2.78}$$

Plugging in to (2.77) and solving for the coefficients gives

$$c_1 = \frac{2\partial_X G_3}{(\xi_0^{\phi,\pm})^2 - 2\sigma\alpha^2|\xi|^2_h}\left[\left(\tfrac{2\sigma-1}{4}D^k\phi D_k\phi - (6\sigma+1)K_\phi^2\right)\hat{a}^\phi + 2\sigma K_\phi \xi_k D^k\phi\, \hat{\phi}\right] \tag{2.79}$$

$$c_2 = -\frac{1}{|\xi|^2_h}\partial_X G_3 X \hat{a}^\phi \tag{2.80}$$

$$c_3 = -\partial_X G_3 \hat{a}^\phi \tag{2.81}$$

$$c_4 = \partial_X G_3 K_\phi \hat{\phi} \tag{2.82}$$

In order for c_1 to be smooth for any nonzero ξ_i, $-(\xi_0^{\phi,\pm})^2 + 2\sigma\alpha^2|\xi|^2_h$ must be nonzero for any ξ_i. This can be achieved by choosing σ to be large enough. To see why this is true, we first note that the zeros of the function

$$\mathcal{F}_\sigma(\xi_0;\xi_i) = -(\xi_0)^2 + 2\sigma\alpha^2|\xi|^2_h \tag{2.83}$$

define a cone for any $\sigma > 0$, a null cone of a Lorentzian metric. In the weakly coupled regime (see (2.24)), the null cone of $P'_{\phi\phi}$ is a small deformation of the null cone of the spacetime metric g for any ξ_i, they might even intersect for special values of ξ_i (and for particular field configurations). Recall that

$$g^{\mu\nu}\xi_\mu\xi_\nu = -(\xi_0)^2 + \alpha^2|\xi|^2_h = \mathcal{F}_{\sigma=1/2}(\xi_0;\xi_i), \tag{2.84}$$

i.e., when $\sigma = 1/2$ is a constant function, the null cone $\mathcal{F}_\sigma = 0$ coincides with the null cone of the spacetime metric. This implies that the expression on the RHS of (2.79) could blow up for some ξ_i when $\sigma = \frac{1}{2}$. To avoid this, we can just choose σ to be any function that takes up values larger than (or smaller than) 1/2, so that the cone given by $\mathcal{F}_\sigma(\xi_0;\xi_i) = 0$ lies entirely “inside” (or "outside") the null cones of g and $P'_{\phi\phi}$ at the cotangent space of any point in spacetime. In other words, for an appropriate $\sigma > \frac{1}{2}$ (or $\sigma < \frac{1}{2}$), the function $\mathcal{F}_\sigma(\xi_0^{\phi,\pm};\xi_i)$ vanishes for no choice of ξ_i. For larger values of $|\sigma - 1/2|$, the BSSN system may be strongly hyperbolic for stronger Horndeski couplings because for such choices of σ the null cone of $P'^{\mu\nu}_{\phi\phi}$ is allowed to deviate more from the null cone of $g^{\mu\nu}$ without intersecting the cone $\mathcal{F}_\sigma(\xi_0;\xi_i) = 0$.

To summarize, we have shown that the equations of motion for cubic Horndeski theories form a strongly hyperbolic system in a version of the BSSN formulation, under the assumption that the Horndeski terms are sufficiently small compared to the Einstein-scalar-field terms (i.e. at small couplings). The system was obtained using a generalization of the harmonic slicing condition and an arbitrary but (nondynamically) fixed shift vector. The system is strongly hyperbolic for any $p > \frac{1}{4}$ and for suitable choice of the function $\sigma \equiv \partial_K F$ that takes up values sufficiently larger or smaller than 1/2. (At weak couplings, choosing a constant, e.g. $\sigma = 1$ is enough.) This means that the original harmonic slicing $\sigma = \frac{1}{2}$ does not work for cubic Horndeski theories. On the other hand, the so-called 1+log slicing often used in numerical relativity, corresponds to the choice $\sigma = \frac{1}{\alpha}$ and hence remains a good slicing condition as long as $\alpha < 2$.

To complete the proof of well-posedness, we continue the discussion with constraint propagation.

2.3.3 Propagation of constraints

To show that the solutions of the BSSN system are also solutions of the original Horndeski equations of motion, we derive a system of evolution equations for the Hamiltonian constraint, the momentum constraint and the variable

$$\tilde{\mathbf{W}}^k \equiv \tilde{V}^k + \mathring{D}_l \tilde{h}^{kl}; \tag{2.85}$$

and show that the system of equations is strongly hyperbolic. By uniqueness of the solutions to strongly hyperbolic systems, it follows that if the constraints are satisfied initially then they continue to hold throughout the evolution.

Starting from equations (2.36) and (2.37) and setting

$$\mathcal{E}_{ij} \to \mathcal{E}_{ij} - \alpha \left(\tilde{h}_{k(i}\partial_{j)}\tilde{\mathbf{W}}^k\right)^{TF} + \frac{2}{3}\alpha \mathbf{H}\, h_{ij}, \tag{2.86}$$

the constraint evolution equations become

$$\begin{aligned}(\partial_t - \mathcal{L}_\beta)\,\mathbf{H} \quad = \quad & \frac{2}{3}\alpha K\mathbf{H} + \frac{1}{\alpha}D^i\left(\alpha^2\mathbf{M}_i\right) - \alpha e^{-4\Omega}\tilde{A}^{ij}\tilde{h}_{k(i}\partial_{j)}\tilde{\mathbf{W}}^k \\ & +2\alpha\partial_X G_3 K_\phi \Bigg[16\mathbf{H}K_\phi^2 + 4K_\phi \mathbf{M}_i D^i\phi \\ & + \left(-\left(\tilde{h}_{k(i}\partial_{j)}\tilde{\mathbf{W}}^k\right)^{TF} + \frac{2}{3}\mathbf{H}h_{ij}\right) D^i\phi D^j\phi\Bigg]\end{aligned} \tag{2.87a}$$

$$\begin{aligned}(\partial_t - \mathcal{L}_\beta)\,\mathbf{M}_i &= \alpha K\mathbf{M}_i - \frac{\alpha^3}{3}D^i\left(\alpha^{-2}\mathbf{H}\right) - D^j\left[\alpha\left(\tilde{h}_{k(i}\partial_{j)}\tilde{\mathbf{W}}^k\right)^{TF}\right] \\ &\quad -\alpha\partial_X G_3 D_i\phi\Bigg[16\mathbf{H}K_\phi^2 + 4K_\phi\mathbf{M}_i D^i\phi \\ &\quad +\left(-\left(\tilde{h}_{k(i}\partial_{j)}\tilde{\mathbf{W}}^k\right)^{TF} + \frac{2}{3}\mathbf{H}h_{ij}\right)D^i\phi D^j\phi\Bigg] \end{aligned} \tag{2.87b}$$

$$(\partial_t - \mathcal{L}_\beta)\,\tilde{\mathbf{W}}^i = -2\alpha p\tilde{h}^{ij}\mathbf{M}_j. \tag{2.87c}$$

We remind the reader that indices of tensors whose notation involves a tilde are raised and lowered with the conformal metric $\tilde{h}$, indices of tensors without a tilde are raised and lowered with the original induced metric h.

Note that we have two additional constraints: the tracelessness of $\tilde{A}_{ij}$ and $\det\mathring{h} = \det\tilde{h}$. Introducing the constraint variables

$$\mathbf{T} \equiv \tilde{h}^{ij}\tilde{A}_{ij} \tag{2.88}$$

and

$$\mathbf{D} \equiv \ln\frac{\det\tilde{h}}{\det\mathring{h}}, \tag{2.89}$$

it follows easily that

$$\partial_0\mathbf{T} = -\frac{1}{2}e^{-4\Omega}\tilde{h}^{ij}\mathring{D}_i\mathring{D}_j\mathbf{D} \tag{2.90}$$

and

$$\partial_0\mathbf{D} = -2\mathbf{T}. \tag{2.91}$$

Substituting (2.90) into the time derivative of (2.91) implies a wave equation for $\mathbf{D}$, decoupled from the rest of the constraint propagation system (2.87):

$$\partial_0^2\mathbf{D} = e^{-4\Omega}\tilde{h}^{ij}\mathring{D}_i\mathring{D}_j\mathbf{D}. \tag{2.92}$$

Hence, starting from initial data that satisfies $\mathbf{D} = 0$ and $\mathbf{T} = 0$, these conditions will continue to hold throughout the evolution. In other words, the evolution of these two constraints decouple from the system (2.87) so it remains to study (2.87).

The system (2.87) has the same form as (1.75)-(1.76) with $u = \mathbf{W}^i$ and $v = (\mathbf{H}, \mathbf{M}^i)$. Thus the methods of section (1.2.5) apply here as well. The rows of the characteristic equation read as

$$\xi_0\hat{\mathbf{H}} = \alpha\xi^i\hat{\mathbf{M}}_i, \tag{2.93a}$$

$$\xi_0 \hat{\mathbf{M}}_i = -\frac{1}{3}\alpha\xi_i \mathbf{H} - \frac{1}{2}\alpha|\xi|_h^2 \hat{\tilde{\mathbf{W}}}_i - \frac{1}{6}\alpha\xi_i\xi_j \hat{\tilde{\mathbf{W}}}^j, \tag{2.93b}$$

$$\xi_0 \hat{\tilde{\mathbf{W}}}_i = -2\alpha p \hat{\mathbf{M}}_i \tag{2.93c}$$

where we simply denoted the components of the polarization vector U associated with the variables $\mathbf{W}_i$, $\mathbf{H}$ and $\mathbf{M}_i$ by $\hat{\mathbf{W}}_i$, $\hat{\mathbf{H}}_i$ and $\hat{\mathbf{M}}_i$, respectively. The associated eigenvalues and eigenvectors are as follows.

I. For $\xi_0 = 0$, we have

$$\begin{pmatrix} \hat{\mathbf{H}} \\ \hat{\tilde{\mathbf{W}}}_i \\ \hat{\mathbf{M}}_i \end{pmatrix} = \begin{pmatrix} -2\alpha|\xi|_h^2 \\ \alpha\xi_i \\ 0 \end{pmatrix}. \tag{2.94}$$

II. The eigenvectors corresponding to eigenvalues $\xi_0 = \pm\sqrt{\frac{4p-1}{3}}\alpha|\xi|_h$ are

$$\begin{pmatrix} \hat{\mathbf{H}} \\ \hat{\tilde{\mathbf{W}}}_i \\ \hat{\mathbf{M}}_i \end{pmatrix} = \begin{pmatrix} -\alpha|\xi|_h^2 \\ 2\alpha p\xi_i \\ -\xi_0\xi_i \end{pmatrix}. \tag{2.95}$$

III. Finally, the eigenvectors corresponding to the eigenvalues $\xi_0 = \pm\sqrt{p}\alpha|\xi|_h$ are

$$\xi_0 = \pm\sqrt{p}\alpha|\xi|_h; \quad \begin{pmatrix} \hat{\mathbf{H}} \\ \hat{\tilde{\mathbf{W}}}_i \\ \hat{\mathbf{M}}_i \end{pmatrix} = \begin{pmatrix} 0 \\ 2\alpha p e_i \\ -\xi_0 e_i \end{pmatrix} \tag{2.96}$$

for any vector e_i orthogonal to ξ_i with respect to h_{ij}, i.e., this means a 2-dimensional degenerate eigenspace for both sign choices.

Therefore, we have found a complete set of smooth and bounded eigenvectors with real eigenvalues (provided that $p > \frac{1}{4}$) for the characteristic equation of the system describing the evolution of constraints. Hence, the system of PDEs (2.87) is strongly hyperbolic which concludes the proof of constraint propagation.

2.4 CCZ4-type formulation

2.4.1 Preliminaries and constraints

In this section we discuss how the so-called covariant conformal Z4 (CCZ4) [79, 85–88] formulation extends to the class of theories under consideration. This formulation is currently one of the most widely used numerical schemes due to its favorable stability properties [85, 86].

The idea behind the CCZ4 formulation is to introduce a 4-vector field $\mathcal{Z}^a$ whose role is to measure deviations (due to numerical errors or constraint violations) in a numerical simulation from the actual gravitational equations of motion E_{ab} (see (2.2)). One then adds terms containing $\mathcal{Z}^a$ and its first derivatives to the equations so that $\mathcal{Z}_a = 0$ is an attractor of the modified equations. The modification is carried out in the following way:

$$\begin{aligned} E_{ab} = 0 \to & E_{ab} + \nabla_a \mathcal{Z}_b + \nabla_b \mathcal{Z}_a - g_{ab} \nabla^c \mathcal{Z}_c \\ & - k_1 \left(n_a \mathcal{Z}_b + n_b \mathcal{Z}_a + k_2 n^c \mathcal{Z}_c g_{ab} \right) = 0, \end{aligned} \tag{2.97}$$

or in the trace reversed version

$$\begin{aligned} E_{ab} - \frac{1}{2} E g_{ab} = 0 \to & E_{ab} - \frac{1}{2} E g_{ab} + \nabla_a \mathcal{Z}_b + \nabla_b \mathcal{Z}_a \\ & - k_1 \left(n_a \mathcal{Z}_b + n_b \mathcal{Z}_a - (1 + k_2) n^c \mathcal{Z}_c g_{ab} \right) = 0. \end{aligned} \tag{2.98}$$

The parameters k_1 and k_2 here are real constants. Splitting the four vector $\mathcal{Z}^a$ as $\mathcal{Z}^a \equiv Z^a + n^a \Theta$ with $Z^a \equiv h^a_b \mathcal{Z}^b$ and $\Theta \equiv -n^a \mathcal{Z}_a$, one can write the normal-normal and normal-spatial projections of (2.97) as

$$\begin{aligned} \left(\partial_t - \mathcal{L}_\beta \right) \Theta = & \alpha \mathbf{H} - \alpha \Theta K + \alpha D_k Z^k \\ & - D_k \alpha Z^k - (2 + k_2) k_1 \alpha \Theta, \end{aligned} \tag{2.99}$$

$$\left(\partial_t - \mathcal{L}_\beta \right) Z_i = -\alpha \mathbf{M}_i + \alpha D_i \Theta - D_i \alpha \Theta - 2 K_{ik} Z^k - k_1 Z_i \tag{2.100}$$

where the expressions for the Hamiltonian and momentum constraints ($\mathbf{H}$ and $\mathbf{M}_i$) are given by equations (2.11) and (2.12).

When the generalized Bianchi-identity (2.34) holds, the evolution equations for the Hamiltonian and momentum constraints are

$$
\begin{aligned}
(\partial_t - \mathcal{L}_\beta)\,\mathbf{H} \;=\;& 2\alpha K\mathbf{H} + \frac{1}{\alpha}D^i\left(\alpha^2\mathbf{M}_i\right) - 2\alpha k_1(1+k_2)K\Theta \\
&+2\alpha\left(Kh^{kl} - K^{kl}\right)(D_l Z_k - \Theta K_{kl}) \\
&-4\alpha\partial_X G_3 K_\phi\Big[D^i\phi D^j\phi D_i Z_j + 2D^k Z_k K_\phi^2 - D^i\phi D^j\phi K_{ij}\Theta - 4K\Theta K_\phi^2 \\
&-4\mathbf{H}K_\phi^2 - 2K_\phi \mathbf{M}_i D^i\phi - \frac{1}{2}k_1(1+k_2)(12K_\phi^2 + D^k\phi D_k\phi)\Theta\Big] \qquad (2.101)
\end{aligned}
$$

$$
\begin{aligned}
(\partial_t - \mathcal{L}_\beta)\,\mathbf{M}_i \;=\;& \alpha K\mathbf{M}_i + \frac{1}{\alpha}D^i\left(\alpha^2\mathbf{H}\right) \\
&+2D^j\Big[\alpha\Big(D^k Z_k h_{ij} - D_{(i}Z_{j)} + \Theta(K_{ij} - Kh_{ij}) - k_1(1+k_2)\Theta h_{ij}\Big)\Big] \\
&+2\alpha\partial_X G_3 D_i\phi\Big[D^i\phi D^j\phi D_i Z_j + 2D^k Z_k K_\phi^2 - D^i\phi D^j\phi K_{ij}\Theta \\
&\qquad -4\mathbf{H}K_\phi^2 + 4K\Theta K_\phi^2 - 2K_\phi\mathbf{M}_i D^i\phi \\
&\qquad -\frac{1}{2}k_1(1+k_2)(12K_\phi^2 + D^k\phi D_k\phi)\Theta\Big]. \qquad (2.102)
\end{aligned}
$$

Once again, the system (2.99-2.102) describing the propagation of constraint violations has the same principal symbol as in general relativity, cf. equations (7), (8), (11), (12) of [89]. Therefore, the hyperbolicity and the high frequency behaviour of that system is not altered by the Horndeski terms. This has the following implications for constraint damping. Similarly to [89], one can carry out a preliminary mode analysis by linearizing around a generic field configuration at weak couplings and studying the high frequency limit of (2.99-2.102). For large frequencies, the Horndeski terms become insignificant. Making a plane wave ansatz for the constraint variables then reduces the high frequency limit of (2.99-2.102) to the same eigenvalue problem as in [89] (see equation (19)). Hence, we come to the same conclusion as in vacuum GR: the real parts of all eigenfrequencies are negative if $k_1 > 0$ and $k_2 > -1$. This suggests that with such choice of the parameters k_1 and k_2, large frequency constraint violating modes will be damped away in cubic Horndeski theories.

2.4.2 Equations of motion

Next, we provide the full system of evolution equations, in the conformal decomposition. We introduce $\tilde{Z}_i \equiv Z_i$, $\tilde{Z}^i \equiv \tilde{h}^{ij}\tilde{Z}_j$ and

$$\tilde{U}^i \equiv h^{kl}\left(\tilde{\Gamma}^i_{kl} - \mathring{\Gamma}^i_{kl}\right) + 2\tilde{Z}^i = \tilde{V}^i + 2\tilde{Z}^i. \tag{2.103}$$

Similarly to the BSSN case, we use auxiliary variables

$$\begin{aligned}
\tilde{\Phi} \equiv \Phi &= -\frac{2}{\alpha}\left(\partial_0 K_\phi + e^{-4\Omega}\tilde{h}^{ij}\tilde{D}_i\phi\tilde{D}_j\alpha\right), && (2.104)\\
\tilde{\Phi}_i \equiv \Phi_i &= -2\tilde{D}_i K_\phi + \tilde{A}_{ik}\tilde{D}_j\phi\tilde{h}^{jk} + \tfrac{1}{3}K\tilde{D}_i\phi, && (2.105)\\
\tilde{\Phi}_{ij} \equiv \Phi_{ij} &= \tilde{D}_i\tilde{D}_j\phi - 2\Big(\tilde{D}_j\phi\tilde{D}_i\Omega + \tilde{D}_i\phi\tilde{D}_j\Omega - \tilde{h}_{ij}\tilde{h}^{kl}\tilde{D}_k\phi\tilde{D}_l\Omega\Big) && (2.106)\\
&\quad -2K_\phi e^{4\Omega}\Big(\tilde{A}_{ij} + \tfrac{1}{3}K\tilde{h}_{ij}\Big), && (2.107)\\
\tilde{\rho} &\equiv e^{4\Omega}\Big(R[D] + \tfrac{2}{3}K^2 - \tilde{A}_{ik}\tilde{A}_{jl}\tilde{h}^{ij}\tilde{h}^{kl}\Big) && (2.108)
\end{aligned}$$

to write the equations more compactly.

We are going to use a natural generalization of the harmonic slicing condition adapted to the CCZ4 system (recall $\partial_0 \equiv \partial_t - \beta^k\mathring{D}_k$)

$$\partial_0\alpha = -2\alpha^2\sigma(t,x,\alpha)(K - 2\Theta). \tag{2.109a}$$

The shift vector is evolved using the standard "Gamma driver" condition [84]

$$\partial_0\beta^i = f(t,x,\alpha)\alpha^2 e^{-4\Omega}B^i \tag{2.109b}$$

$$\partial_0 B^i = \partial_0\tilde{U}^i - \eta(t,x)B^i. \tag{2.109c}$$

In these equations f and η are freely specifiable functions and B^i is an auxiliary variable. The evolution equations for the variables $\tilde{h}_{ij}$ and Ω are just the defining equations (2.45) and (2.46), and are left unaltered:

$$\partial_0\tilde{h}_{ij} = -2\alpha\tilde{A}_{ij} + 2\tilde{h}_{k(i}\mathring{D}_{j)}\beta^k - \frac{2}{3}\tilde{h}_{ij}\mathring{D}_k\beta^k, \tag{2.109d}$$

$$\partial_0\Omega = -\frac{\alpha}{6}K + \frac{1}{6}\mathring{D}_k\beta^k. \tag{2.109e}$$

The evolution equation for Θ is the same as (2.99) (using the expression of the Hamiltonian constraint)

$$\begin{aligned}
\partial_0\Theta &= \tfrac{1}{2}\alpha\Big(\tilde{\rho}e^{-4\Omega} - 2K_\phi^2 - \tfrac{1}{2}e^{-4\Omega}\tilde{D}_i\phi\tilde{D}_j\phi\tilde{h}^{ij} + G_2 \\
&\quad -4K_\phi^2\partial_X G_2 - \partial_\phi G_3\Big(4K_\phi^2 + e^{-4\Omega}\tilde{D}_i\phi\tilde{D}_j\phi\tilde{h}^{ij}\Big) \\
&\quad +\partial_X G_3\Big(-4K_\phi^2 e^{-4\Omega}\tilde{\Phi}_{ij}\ \tilde{h}^{ij} + e^{-8\Omega}\tilde{D}_k\phi\tilde{D}_l\phi\tilde{\Phi}_{ij}\ \tilde{h}^{ik}\tilde{h}^{jl}\Big)\Big) \\
&\quad +\alpha\Big(e^{-4\Omega}\tilde{D}_i\tilde{Z}^i + 2e^{-4\Omega}\tilde{Z}^i\tilde{D}_i\Omega - \Theta K \\
&\qquad -e^{-4\Omega}\tilde{Z}^i\mathring{D}_i\ln\alpha - k_1(2+k_2)\Theta\Big). \qquad (2.109\text{f})
\end{aligned}$$

Equation (2.102) is no longer kept as a separate equation, instead, it is added to the evolution equation for $\tilde{V}^i$:

$$\begin{aligned}
\partial_0\tilde{U}^i &= 2\alpha\Big(-\tfrac{2}{3}\tilde{D}^iK + \tilde{\Gamma}^i_{jk}\tilde{A}^{jk} + 6\tilde{A}^{ij}\tilde{D}_j\Omega + \tilde{D}^i\Theta - \Theta\tilde{D}^i\ln\alpha - \tfrac{2}{3}K\tilde{Z}^i\Big) \\
&\quad -2\tilde{A}^{ij}\tilde{D}_j\alpha - \tilde{U}^k\mathring{D}_k\beta^i + \tfrac{2}{3}\tilde{U}^i\mathring{D}_k\beta^k + \tilde{h}^{kl}\mathring{D}_k\mathring{D}_l\beta^i \\
&\quad +\tfrac{1}{3}\tilde{h}^{ij}\mathring{D}_j\mathring{D}_k\beta^k - 2\alpha k_1\tilde{Z}^i + 2k_3\Big(\tfrac{2}{3}\tilde{Z}^i\mathring{D}_k\beta^k - \tilde{Z}^k\mathring{D}_k\beta^i\Big) \\
&\quad -2N\Big\{\tilde{D}^i\phi K_\phi + \tilde{D}^i\phi K_\phi\partial_X G_2 + 2\tilde{D}^i\phi K_\phi\partial_\phi G_3 \\
&\quad +\tfrac{1}{2}\partial_X G_3\Big(-4K_\phi^2\tilde{\Phi}^i - 2\tilde{D}_k\phi K_\phi\tilde{\Phi}_{jl}\tilde{h}^{kl}\tilde{h}^{ij}e^{-4\Omega} \\
&\quad +2\tilde{D}^i\phi K_\phi\tilde{\Phi}_{kl}\tilde{h}^{kl}e^{-4\Omega} + \tilde{D}_k\phi\tilde{D}^i\phi\tilde{\Phi}_l\ \tilde{h}^{kl}e^{-4\Omega}\Big)\Big\} \qquad (2.109\text{g})
\end{aligned}$$

This is equivalent to adding the momentum constraint times 2α to (2.55). The evolution equations for K and $\tilde{A}_{ij}$ are the same as before, except for the constraint damping terms:

$$\begin{aligned}
0 &= -\partial_0K + \frac{1}{4}\alpha\partial_X G_3(12K_\phi^2 - e^{-4\Omega}\tilde{D}^k\phi\tilde{D}_k\phi)\Phi \\
&\quad +\alpha\Big\{R[D] + 2e^{-4\Omega}\tilde{D}_k\tilde{Z}^k + 4e^{-4\Omega}\tilde{Z}^k\tilde{D}_k\Omega + K^2 - 2\Theta K \\
&\quad +\frac{1}{\alpha}e^{-4\Omega}\Big(\tilde{h}^{ij}\tilde{D}_i\tilde{D}_j\alpha + 2\tilde{h}^{ij}\tilde{D}_i\alpha\tilde{D}_j\Omega\Big) - 3k_1(1+k_2)\Theta \\
&\quad -\frac{1}{2}\tilde{D}_i\phi\tilde{D}_j\phi\tilde{h}^{ij}e^{-4\Omega} - \partial_\phi G_3\tilde{D}_i\phi\tilde{D}_j\phi\tilde{h}^{ij}e^{-4\Omega} \\
&\quad +\frac{3}{2}G_2 + \partial_X G_2\Big(-3K_\phi^2 + \frac{1}{4}\tilde{D}_i\phi\tilde{D}_j\phi\tilde{h}^{ij}e^{-4\Omega}\Big) \\
&\quad +\partial_X G_3 e^{-4\Omega}\Big(-3K_\phi^2\tilde{\Phi}_{ij}\ \tilde{h}^{ij} + 2\tilde{D}_i\phi K_\phi\tilde{\Phi}_j\tilde{h}^{ij} \\
&\quad +\frac{1}{4}\tilde{D}_i\phi\tilde{D}_j\phi\tilde{\Phi}_{kl}\ \tilde{h}^{ij}\tilde{h}^{kl}e^{-4\Omega} + \tilde{D}_i\phi\tilde{D}_j\phi\tilde{\Phi}_{kl}\ \tilde{h}^{ik}\tilde{h}^{jl}e^{-4\Omega}\Big)\Big\} \qquad (2.109\text{h})
\end{aligned}$$

$$
\begin{aligned}
0 \;=\; & -\partial_0\tilde{A}_{ij}+\frac{1}{2}\alpha e^{-4\Omega}\partial_X G_3\left(\tilde{D}_i\phi\tilde{D}_j\phi-\frac{1}{3}\tilde{h}_{ij}\tilde{D}^k\phi\tilde{D}_k\phi\right)\Phi\\
&+\alpha e^{-4\Omega}\Big[R[D]_{ij}+2\tilde{D}_{(i}\tilde{Z}_{j)}-8\tilde{Z}_{(i}\tilde{D}_{j)}\Omega\\
&-\tfrac{1}{\alpha}\tilde{D}_i\tilde{D}_j\alpha+4\tilde{D}_{(i}\Omega\tilde{D}_{j)}\ln\alpha-\frac{1}{2}\Big(1+\partial_X G_2+2\partial_\phi G_3\Big)\tilde{D}_i\phi\tilde{D}_j\phi\\
&+\partial_X G_3\Big(2K_\phi\tilde{D}_{(i}\phi\tilde{\Phi}_{j)}-\tfrac{1}{2}\tilde{D}_i\phi\tilde{D}_j\phi\tilde{\Phi}_{kl}\tilde{h}^{kl}e^{-4\Omega}+\tilde{D}_k\phi\tilde{D}_{(i}\phi\tilde{\Phi}_{j)l}\,\tilde{h}^{kl}e^{-4\Omega}\Big)\Big]^{\mathrm{TF}}\\
&+\alpha(K-2\Theta)\tilde{A}_{ij}-2\alpha\tilde{A}_{ik}\tilde{A}^k{}_j+2\tilde{A}_{k(i}\mathring{D}_{j)}\beta^k-\frac{2}{3}\tilde{A}_{ij}\mathring{D}_k\beta^k. \qquad (2.109\text{i})
\end{aligned}
$$

Finally, we also have a pair of scalar evolution equations: (2.57), (2.58).

We conclude this section with a technical remark. For general relativity, it has been noted that the CCZ4 equations of motion can be derived from an action principle [87] (at least if we ignore the lower order terms with k_1 and k_2). If we insisted on a similar action principle for cubic Horndeski theories, then upon taking the linear combination (2.5) of the gravitational and scalar equations of motion, the resulting equation would contain principal terms from the ADM decomposition of ∇Z. However, for cubic Horndeski theories, it is better to keep equation (2.58) as the scalar evolution equation. It appears that for these theories, it is more useful to introduce the Z-terms at the level of the equations, rather than at the level of the action.

2.4.3 Strong hyperbolicity

We continue by showing that the system of equations (2.109),(2.57), (2.58) is strongly hyperbolic. Once again, this can be done by a straightforward application of the methods presented in 1.2.5. Setting

$$u=(\alpha,\Omega,\beta^i,\tilde{h}_{ij},\phi) \qquad \text{and} \qquad v=(K,\Theta,B^i,\tilde{U}^i,\tilde{A}_{ij},K_\phi) \qquad (2.110)$$

the CCZ4 system takes the form of the system (1.75)-(1.76). In this case, we have $n=12$ and $m=15$.

The next step is to write down the characteristic equation (2.17), and compute the eigenvalues ξ_0 and the corresponding eigenvectors of the system. We will write the components of the eigenvectors U associated with the 27 variables as

$$U=(\hat{\alpha},\hat{\omega},\hat{\beta}^i,\hat{\tilde{\gamma}}_{ij},\hat{\phi};\hat{\kappa},\hat{\theta},\hat{b}^i,\hat{\tilde{u}}^i,\hat{\tilde{q}}_{ij},\hat{a}) \qquad (2.111)$$

in the same order as in (2.110). The rows of the characteristic equation now read as follows:

$$0 = -\xi_0 \hat{\alpha} - 2\alpha^2 \sigma(\hat{\kappa} - 2\hat{\theta}) \tag{2.112a}$$

$$0 = -\xi_0 \hat{\beta}^i + f\alpha^2 e^{-4\Omega} \hat{b}^i \tag{2.112b}$$

$$0 = -\xi_0 \hat{b}^i + \xi_0 \hat{\tilde{u}}^i \tag{2.112c}$$

$$\begin{aligned} 0 \;\; = \;\; & -\xi_0 \hat{\theta} + \frac{1}{2} \alpha e^{-4\Omega} \Big\{ \xi_k \hat{\tilde{u}}^k - 8|\xi|^2_{\tilde{h}} \hat{\omega} \\ & + \partial_X G_3 \hat{\phi} \left(-4K_\phi^2 |\xi|^2_{\tilde{h}} + e^{-4\Omega} \left(\tilde{D}^k \phi \xi_k \right)^2 \right) \Big\} \end{aligned} \tag{2.112d}$$

$$\begin{aligned} 0 \;\; = \;\; & -\xi_0 \hat{\kappa} - \frac{1}{2} \partial_X G_3 (12K_\phi^2 - D_k \phi D^k \phi) \xi_0 \hat{a} \\ & + \alpha e^{-4\Omega} \Big\{ -\frac{1}{\alpha} |\xi|^2_{\tilde{h}} \hat{\alpha} + \xi_k \hat{\tilde{u}}^k - 8|\xi|^2_{\tilde{h}} \hat{\omega} \\ & - \partial_X G_3 \Big[\frac{1}{4} (12K_\phi^2 - D^k \phi D_k \phi) |\xi|^2_{\tilde{h}} \hat{\phi} \\ & - \left(4K_\phi \hat{a} - \left(\xi_k \tilde{D}^k \phi \right) \hat{\phi} \right) \left(\xi_l \tilde{D}^l \phi \right) \Big] \Big\} \end{aligned} \tag{2.112e}$$

$$0 = -\xi_0 \hat{\omega} - \frac{\alpha}{6} \hat{\kappa} + \frac{1}{6} \xi_k \hat{\beta}^k \tag{2.112f}$$

$$0 = -\xi_0 \hat{\psi} - 2\alpha \hat{a} \tag{2.112g}$$

$$0 = -\xi_0 \hat{\tilde{\gamma}}_{ij} - 2\alpha \hat{\tilde{q}}_{ij} + 2 \left(\xi_{(i} \hat{\beta}_{j)} \right)^{\mathrm{TF}} \tag{2.112h}$$

$$\begin{aligned} 0 \;\; = \;\; & -\xi_0 \hat{\tilde{u}}^i + |\xi|^2_{\tilde{h}} \hat{\beta}^i + \frac{1}{3} \xi^i \xi_k \hat{\beta}^k \\ & + \alpha \Big[-\frac{4}{3} \xi^i \hat{\kappa} + 2\xi^i \hat{\theta} - 8 \partial_X G_3 K_\phi^2 \, \xi^i \hat{a} \\ & \quad + 2e^{-4\Omega} \partial_X G_3 \Big(K_\phi \tilde{D}^k \phi \; \xi_k \xi^i \hat{\phi} \\ & \quad - K_\phi \tilde{D}^i \phi |\xi|^2_{\tilde{h}} \hat{\phi} + \tilde{D}^i \phi \tilde{D}^k \phi \; \xi_k \hat{a} \Big) \Big]. \end{aligned} \tag{2.112i}$$

$$
\begin{aligned}
0 \;=\; & -\xi_0\hat{\tilde{q}}_{ij} - e^{-4\Omega}\partial_X G_3\left(\tilde{D}_i\phi\tilde{D}_j\phi - \frac{1}{3}\tilde{h}_{ij}\tilde{D}^k\phi\tilde{D}_k\phi\right)\xi_0\hat{a} \\
& +\alpha e^{-4\Omega}\Bigg\{-\frac{1}{2}|\xi|^2_{\tilde{h}}\hat{\tilde{\gamma}}_{ij} + \xi_{(i}\hat{\tilde{u}}_{j)} - \frac{1}{3}\xi_k\hat{\tilde{u}}^k\tilde{h}_{ij} \\
& -2\xi_i\xi_j\hat{\omega} + \frac{2}{3}|\xi|^2_{\tilde{h}}\hat{\omega}\tilde{h}_{ij} - \frac{1}{\alpha}\xi_i\xi_j\hat{\alpha} + \frac{1}{3\alpha}|\xi|^2_{\tilde{h}}\hat{\alpha}\tilde{h}_{ij} \\
& +4K_\phi\partial_X G_3\hat{a}\left(\tilde{D}_{(i}\phi\;\xi_{j)} - \frac{1}{3}\tilde{D}^k\phi\;\xi_k\tilde{h}_{ij}\right) \\
& -e^{-4\Omega}\partial_X G_3\hat{\phi}\Bigg(\frac{1}{2}(\tilde{D}_i\phi\tilde{D}_j\phi - \frac{1}{3}\tilde{h}_{ij}\tilde{D}^k\phi\tilde{D}_k\phi)|\xi|^2_{\tilde{h}} \\
& -\tilde{D}^k\phi\tilde{D}_{(i}\phi\xi_{j)}\xi_k + \frac{1}{3}\tilde{D}^k\phi\tilde{D}^l\phi\;\xi_k\xi_l\tilde{h}_{ij}\Bigg)\Bigg\}
\end{aligned}
\tag{2.112j}
$$

$$
0 = -\xi_0\mathcal{A}\hat{a} + \mathcal{B}\hat{a} + \mathcal{C}\hat{\phi} \tag{2.112k}
$$

where, again, we do not need to deal with the precise expressions of the coefficients $\mathcal{A}$, $\mathcal{B}$ and $\mathcal{C}$, we only need to keep in mind that substituting (2.155b) into (2.155d) yields

$$
\hat{\phi}\left(P'_{\phi\phi}\right)^{\mu\nu}\xi_\mu\xi_\nu = 0, \tag{2.113}
$$

i.e., equation (2.21).

Our strategy is analogous to the one described in section 2.3: it is easy to find 25 eigenvalues and eigenvectors of the system (2.112) with $\hat{\phi} = \hat{a} = 0$. For a more compact notation, we use $\bar{\xi}_0$ (see equation (2.67)) instead of ξ_0 to list the eigenvalues:

I. 12 independent modes for arbitrary $\hat{\tilde{\gamma}}_{ij}$ and $\hat{\alpha} = \hat{\omega} = \hat{\beta}^i = \hat{\tilde{u}}^i = 0$, with eigenvalues $\bar{\xi}_0 = \pm 1$.

II. 2 independent modes for arbitrary $\hat{\tilde{\gamma}}_{ij}$ and nontrivial $\hat{\alpha}$, $\hat{\omega}$, $\hat{\beta}^i$, $\hat{\tilde{u}}^i$, with eigenvalues $\bar{\xi}_0 = \pm 1$.

III. 3 independent zero speed modes ($\bar{\xi}_0 = 0$) for arbitrary $\hat{\tilde{u}}^i$.

IV. 2 independent modes with eigenvalues $\bar{\xi}_0 = \pm\sqrt{2\sigma}$.

V. 4 independent modes with $\bar{\xi}_0 = \pm\sqrt{f}$, for arbitrary e^i orthogonal to ξ^i (w.r.t. $\tilde{h}_{ij}$).

VI. 2 independent modes with $\bar{\xi}_0 = \pm\sqrt{\frac{4f}{3}}$.

The full expressions of the corresponding eigenvectors are given in Table 2.2. Clearly, these expressions depend smoothly on ξ_i if $f > 0$ and $\sigma > 0$.

	$\hat{\alpha}$	$\hat{\omega}$	$\hat{\beta}^i$	$\hat{\tilde{\gamma}}_{ij}$	$\bar{\xi}_0$
I.	0	0	0	$\hat{\tilde{\gamma}}_{ij}$	± 1
II.	0	$\mp\frac{\lvert\xi\rvert_{\tilde{h}} e^{-2\Omega}(f-1)}{2f\alpha}$	ξ^i	$\hat{\tilde{\gamma}}_{ij}$	± 1
III.	0	$\frac{1}{8\lvert\xi\rvert^2_{\tilde{h}}}\xi_k \hat{\tilde{u}}^k$	0	$\frac{2}{\lvert\xi\rvert^2_{\tilde{h}}}\left(\xi_{(i}\hat{\tilde{u}}_{j)} - \frac{\xi_i\xi_j}{4\lvert\xi\rvert^2_{\tilde{h}}}\xi_k\hat{\tilde{u}}^k\right)^{\mathrm{TF}}$	0
IV.	$\pm\frac{\sqrt{2\sigma}e^{2\Omega}\lvert\xi\rvert_{\tilde{h}}(3\sigma-2f)}{2f}$	$\pm\frac{\sqrt{2\sigma}e^{2\Omega}\lvert\xi\rvert_{\tilde{h}}}{8\alpha f}$	ξ^i	$\pm\frac{3\sqrt{2\sigma}e^{2\Omega}}{2f\alpha\lvert\xi\rvert_{\tilde{h}}}\left(\xi_i\xi_j\right)^{\mathrm{TF}}$	$\pm\sqrt{2\sigma}$
V.	0	0	e^i	$\pm\frac{2e^{2\Omega}}{\alpha\sqrt{f}\lvert\xi\rvert_{\tilde{h}}}\xi_{(i}e_{j)}$	$\pm\sqrt{f}$
VI.	0	$\pm\frac{e^{2\Omega}}{4\sqrt{3f}\alpha\lvert\xi\rvert_{\tilde{h}}}$	ξ^i	$\pm\frac{\sqrt{3}\ e^{2\Omega}}{\alpha\sqrt{f}\lvert\xi\rvert_{\tilde{h}}}\left(\xi_i\xi_j\right)^{\mathrm{TF}}$	$\pm\sqrt{\frac{4f}{3}}$

	$\hat{\theta}$	$\hat{\kappa}$	$\hat{\tilde{q}}_{ij}$	$\hat{\tilde{u}}_i$
I.	0	0	$\mp\frac{1}{2}\lvert\xi\rvert_{\tilde{h}}e^{-2\Omega}\hat{\tilde{\gamma}}_{ij}$	0
II.	$\frac{\lvert\xi\rvert^2_{\tilde{h}}e^{-4\Omega}(4f-3)}{2f\alpha}$	$\frac{\lvert\xi\rvert^2_{\tilde{h}}e^{-4\Omega}(4f-3)}{f\alpha}$	$\mp\frac{1}{2}\lvert\xi\rvert_{\tilde{h}}e^{-2\Omega}\hat{\tilde{\gamma}}_{ij} + \frac{1}{\alpha}\left(\xi_i\xi_j\right)^{\mathrm{TF}}$	$\pm\frac{\lvert\xi\rvert_{\tilde{h}}e^{2\Omega}}{\alpha f}\xi_i$
III.	0	0	0	$\hat{\tilde{u}}_i$
IV.	0	$\frac{2f-3\sigma}{2f\alpha}\lvert\xi\rvert^2_{\tilde{h}}$	$\frac{2f-3\sigma}{2f\alpha}\left(\xi_i\xi_j\right)^{\mathrm{TF}}$	$\pm\sqrt{2\sigma}\frac{\lvert\xi\rvert_{\tilde{h}}e^{2\Omega}}{\alpha f}\xi_i$
V.	0	0	0	$\pm\frac{\lvert\xi\rvert_{\tilde{h}}e^{2\Omega}}{\alpha\sqrt{f}}e_i$
VI.	0	0	0	$\pm\frac{2\lvert\xi\rvert_{\tilde{h}}e^{2\Omega}}{\alpha\sqrt{3f}}\xi_i$

Table 2.2 The list of eigenvalues and eigenvectors with $\hat{\phi} = \hat{a} = 0$.

To show that the system consisting of equations (2.109), (2.57), (2.58) is strongly hyperbolic, it remains to be shown that (2.112) has two eigenvectors corresponding to the eigenvalues $\xi_0^{\phi,\pm}$ (obtained by solving (2.21)), with smooth dependence on ξ_i, with nonzero $\hat{\phi}$ and $\hat{a}^\phi \equiv -\frac{2}{\alpha}\xi_0^{\phi,\pm}\hat{\phi}$ (see equation (2.112g)). These eigenvectors can be found as follows. Recall the general form of the characteristic equation (2.17) from Section 2.2. When separating the terms in the characteristic equations (2.112) to Einstein-scalar-field and Horndeski parts (terms containing a factor $\partial_X G_3$) as in (2.20), we see that the Horndeski terms only act on the $\hat{\phi}$, $\hat{a}$ components of U. In other words, the matrices $\delta\mathbb{A}$ and $\delta\mathbb{L}$ in (2.20) are projections to the subspace associated with the scalar variables:

$$\begin{aligned}
\delta\mathbb{A}\ U &\equiv \delta\mathbb{A}\ (\hat{\alpha},\hat{\omega},\hat{\theta},\hat{\kappa},\hat{\beta}^i,\hat{b}^i,\hat{\tilde{u}}^i,\hat{\tilde{\gamma}}_{ij},\hat{\tilde{q}}_{ij},\hat{\phi},\hat{a})^T \\
&= \delta\mathbb{A}\ (0_{25},\hat{\psi},\hat{a})^T, \qquad (2.114)\\
\delta\mathbb{L}\ U &\equiv \delta\mathbb{L}\ (\hat{\alpha},\hat{\omega},\hat{\theta},\hat{\kappa},\hat{\beta}^i,\hat{b}^i,\hat{\tilde{u}}^i,\hat{\tilde{\gamma}}_{ij},\hat{\tilde{q}}_{ij},\hat{\phi},\hat{a})^T \\
&= \delta\mathbb{L}\ (0_{25},\hat{\phi},\hat{a})^T. \qquad (2.115)
\end{aligned}$$

The eigenvectors $U^{\phi,\pm}$ corresponding to the eigenvalues $\xi^{\pm,\phi}$ then satisfy

$$\begin{aligned}
\left(\xi_0^{\pm,\phi}\mathbb{A}_0 - \mathbb{L}_0(\xi_k)\right)U^{\phi,\pm} &= -\left(\xi_0^{\pm,\phi}\delta\mathbb{A}_0 - \delta\mathbb{L}_0(\xi_k)\right)U^{\phi,\pm} \\
&= -\left(\xi_0^{\pm,\phi}\delta\mathbb{A}_0 - \delta\mathbb{L}_0(\xi_k)\right)\left(0_{25},\hat{\phi},\hat{a}^\phi\right)^T \qquad (2.116)
\end{aligned}$$

where we used (2.20) in the first step and equations (2.114)-(2.115) in the second step. We can find the rest of the components of $U^{\phi,\pm}$ by solving the linear system of equations (2.116) for the variables $(\hat{\alpha},\hat{\omega},\hat{\theta},\hat{\kappa},\hat{\beta}^i,\hat{b}^i,\hat{\tilde{u}}^i,\hat{\tilde{\gamma}}_{ij},\hat{\tilde{q}}_{ij})$. Before doing this, let us introduce the notation $\tilde{T}_{\cdot\xi}$ for the contraction $\tilde{T}_{\cdot i}\xi_j\tilde{h}^{ij}$. Furthermore, let us introduce a basis of vectors $\{e_1^i, e_2^i, e_3^i\}$ tangent to hypersurfaces of $t = $ constant so that e_1 is aligned with ξ^i. We define indices $I, J, ...$ that take values 2 or 3, i.e. they are associated with the subspace orthogonal to ξ^i (w.r.t. the metric h). A straightforward but lengthy calculation gives the formal solution of (2.116):

$$\begin{aligned}
\hat{\alpha}_{\phi,\pm} = &-\frac{\partial_X G_3 \alpha\sigma\hat{\phi}}{2\left((\xi_0^{\pm,\phi})^2 - 2\sigma\alpha^2|\xi|^2_{\tilde{h}}e^{-4\Omega}\right)}\Big[(12K_\phi^2 - \tilde{D}^k\phi\tilde{D}_k\phi e^{-4\Omega})(\xi_0^{\pm,\phi})^2 \\
&+\alpha^2 e^{-4\Omega}\Big(\left(4K_\phi^2 + \tilde{D}^k\phi\tilde{D}_k\phi e^{-4\Omega}\right)|\xi|^2_{\tilde{h}} + 8\alpha K_\phi\tilde{D}^k\phi\xi_k\xi_0^{\pm,\phi}\Big)\Big], \qquad (2.117\text{a})
\end{aligned}$$

$$\hat{\theta}_{\phi,\pm} = 0, \tag{2.117b}$$

$$\begin{aligned}\hat{\kappa}_{\phi,\pm} = \frac{\partial_X G_3 \xi_0^{\pm,\phi} \hat{\phi}}{4\alpha \left((\xi_0^{\pm,\phi})^2 - 2\sigma\alpha^2 |\xi|^2_{\tilde{h}} e^{-4\Omega} \right)} \Big[&(12K_\phi^2 - \tilde{D}^k\phi \tilde{D}_k\phi e^{-4\Omega})(\xi_0^{\pm,\phi})^2 \\ &+ \alpha^2 e^{-4\Omega} \Big(\left(4K_\phi^2 + \tilde{D}^k\phi\tilde{D}_k\phi e^{-4\Omega} \right) |\xi|^2_{\tilde{h}} + 8\alpha K_\phi \tilde{D}^k\phi \xi_k \xi_0^{\pm,\phi} \Big) \Big],\end{aligned} \tag{2.117c}$$

$$\begin{aligned}\hat{\beta}_\xi^{\phi,\pm} = &\frac{\alpha^2 f \xi_0^{\pm,\phi} |\xi|^2_{\tilde{h}} \hat{\phi} \partial_X G_3 e^{-8\Omega}}{3\left((\xi_0^{\pm,\phi})^2 - 2\sigma\alpha^2|\xi|^2_{\tilde{h}} e^{-4\Omega} \right)\left(-(\xi_0^{\pm,\phi})^2 + \frac{4}{3} f\alpha^2 |\xi|^2_{\tilde{h}} e^{-4\Omega} \right)} \\ &\times \Big[3\left(\tilde{A}_\xi^2 e^{-4\Omega} - \tilde{D}^k\phi\tilde{D}_k\phi \right)(\xi_0^{\pm,\phi})^2 + 8\alpha K_\phi \tilde{D}_k\phi\ \xi^k \xi_0^{\pm,\phi} \\ &+ \alpha^2 |\xi|^2_{\tilde{h}} \left(4(6\sigma+1)K_\phi^2 + \tilde{D}^k\phi\tilde{D}_k\phi\ e^{-4\Omega} - 6\sigma e^{-8\Omega}(\xi^k\tilde{D}_k\phi)^2 \right) \Big],\end{aligned} \tag{2.117d}$$

$$\hat{\beta}_I^{\phi,\pm} = \frac{\tilde{D}_I\phi e^{-8\Omega}\ f\alpha^2 \hat{\phi} \partial_X G_3 \left(2\alpha K_\phi |\xi|^2_{\tilde{h}} + \xi^k \tilde{D}_k\phi\ \xi_0^{\pm,\phi} \right)}{\left(-(\xi_0^{\pm,\phi})^2 + f\alpha^2|\xi|^2_{\tilde{h}} e^{-4\Omega} \right)}, \tag{2.117e}$$

$$\begin{aligned}\hat{\hat{u}}_\xi^{\phi,\pm} = \hat{b}_\xi^{\phi,\pm} = \frac{\xi_0^{\pm,\phi} e^{4\Omega}}{f\alpha^2} \hat{\beta}_\xi^{\phi,\pm}, \\ \hat{\hat{u}}_I^{\phi,\pm} = \hat{b}_I^{\phi,\pm} = \frac{\xi_0^{\pm,\phi} e^{4\Omega}}{f\alpha^2} \hat{\beta}_I^{\phi,\pm},\end{aligned} \tag{2.117f}$$

$$\begin{aligned}\hat{\hat{q}}_{ij}^{\phi,\pm} = &\frac{1}{2} \partial_X G_3 \xi_0^{\pm,\phi} \left(\tilde{D}_i\phi\tilde{D}_j\phi - \tfrac{1}{3}\tilde{D}^k\phi\tilde{D}_k\phi\tilde{h}_{ij} \right)\hat{\phi} \\ &+ 2\partial_X G_3 K_\phi \left(\tilde{D}_{(i}\phi\ \xi_{j)} - \tfrac{1}{3}\tilde{D}_k\phi\ \xi^k \tilde{h}_{ij} \right)\hat{\phi} \qquad (2.117g) \\ &+ \frac{\partial_X G_3 \left(\xi_i\xi_j - \frac{1}{3}|\xi|^2_{\tilde{h}}\tilde{h}_{ij} \right)\hat{\phi}}{-(\xi_0^{\phi,\pm})^2 + 2\sigma\alpha^2|\xi|^2_{\tilde{h}}} \Big[-4\sigma K_\phi \tilde{D}_k\phi\ \xi^k e^{-4\Omega} \\ &+ \left(-(6\sigma+1)K_\phi^2 + \frac{2\sigma-1}{4}\tilde{D}^k\phi\tilde{D}_k\phi\ e^{-4\Omega} \right)\xi_0^{\pm,\phi} \Big],\end{aligned} \tag{2.117h}$$

$$\hat{\hat{\gamma}}_{ij}^{\phi,\pm} = \frac{1}{\xi_0^{\pm,\phi}} \left(-2\alpha\hat{\hat{q}}_{ij}^{\phi,\pm} + 2\xi_{(i}\beta_{j)}^{\phi,\pm} - \tfrac{2}{3}\beta_\xi^{\phi,\pm} \right), \tag{2.117i}$$

$$\hat{\omega}_{\phi,\pm} = \frac{1}{6\xi_0^{\pm,\phi}} \left(-\alpha\hat{\kappa}_{\phi,\pm} + \beta_\xi^{\phi,\pm} \right). \tag{2.117j}$$

Interestingly, the θ components of these two eigenvectors are 0. However, this is not surprising at all. This variable measures the constraint violations. But these two eigenvectors correspond to a physical degree of freedom and as such, they must satisfy the high frequency version of the constraints.

In order to avoid singularities in the expressions (2.117) we need to choose the functions σ and f in such a way that the expressions appearing in the denominators

$$-\left(\xi_0^{\phi,\pm}\right)^2 + \frac{4}{3} f \alpha^2 |\xi|^2_{\tilde{h}} e^{-4\Omega}$$

$$-\left(\xi_0^{\phi,\pm}\right)^2 + f \alpha^2 |\xi|^2_{\tilde{h}} e^{-4\Omega}$$

$$-\left(\xi_0^{\phi,\pm}\right)^2 + 2\sigma \alpha^2 |\xi|^2_{\tilde{h}} e^{-4\Omega}$$

are nonzero for all unit covectors ξ_i. This criterion constrains the functions σ and f. To find these constraints, we proceed very similarly to section 2.3.2. Recall that

$$g^{\mu\nu}\xi_\mu\xi_\nu = -(\xi_0)^2 + \alpha^2|\xi|^2_h \tag{2.118}$$

and the fact that the roots $\xi_0^{\phi,\pm}$ are found by solving $P'^{\mu\nu}_{\phi\phi}\xi_\mu\xi_\nu = 0$ for ξ_0 at fixed ξ_i. However, at weak couplings, the null cone of $P'_{\phi\phi}$ is a slightly distorted version of the null cone of the spacetime metric g. Since $P'_{\phi\phi}$ depends on the scalar field and its derivatives up to second order, there might exist a covector ξ_i such that $-(\xi_0^{\phi,\pm})^2 + \alpha^2|\xi|^2_h = 0$ for some field configurations. In other words, the null cones of g and $P'_{\phi\phi}$ may intersect. This means that the expressions (2.117) may fail to have smooth dependence on ξ_i for some choices of ξ_i if $\sigma = \frac{1}{2}$, $f = \frac{3}{4}$ or $f = 1$. We can avoid this by choosing the functions σ and f such that one of the following inequalities holds

(i) $\sigma > \frac{1}{2}$ and $f > 1$,

(ii) $\sigma < \frac{1}{2}$ and $f > 1$,

(iii) $\sigma > \frac{1}{2}$ and $f < \frac{3}{4}$,

(iv) $\sigma < \frac{1}{2}$ and $f < \frac{3}{4}$.

The CCZ4 system may be strongly hyperbolic for larger couplings if one chooses larger values of $|\sigma - 1/2|$ and $|f - 1|$ in cases (i)-(ii), or if the functions $|\sigma - 1/2|$ and $|f - 3/4|$ take larger values in cases (iii)-(iv). In particular, the combination of the 1+log slicing ($\sigma = \frac{1}{\alpha}$, $\alpha < 2$) and a Gamma driver shift condition with a constant function $f > 1$ appears to be a good candidate for numerical relativity simulations.

Appendix 2.A Elliptic-Hyperbolic formulation

In this Appendix, we discuss an additional well-posed formulation of the cubic Horndeski equations of motion. This is an extention of previous work on rewriting Einstein's equations as a coupled system of elliptic and hyperbolic equations [80]. This approach may not be well-suited to numerical relativity implementations due to the high computational cost of solving elliptic PDEs. Nonetheless, it may be of interest from a mathematical point of view.

2.A.1 Review of Andersson and Moncrief's results

In this subsection we briefly summarize the work done by Andersson and Moncrief [80] on the vacuum Einstein's equations. Firstly, we describe how they derived a coupled elliptic-hyperbolic system equivalent to the vacuum Einstein's equations. Then we sketch their arguments establishing local well-posedness.

We start from the ADM formulation in which the vacuum Einstein equations

$$R_{ab} = 0 \tag{2.119}$$

are rewritten as two sets of first order in time evolution equations

$$\left(\partial_t - \mathcal{L}_\beta\right) h_{ij} = -2\alpha K_{ij} \tag{2.120a}$$

$$\left(\partial_t - \mathcal{L}_\beta\right) K_{ij} = -D_i D_j \alpha + \alpha \left(R[D]_{ij} + K K_{ij} - 2K_{ik}K^k_j\right), \tag{2.120b}$$

complemented by the Hamiltonian constraint

$$2\mathbf{H} \equiv 2E_{\mu\nu}n^\mu n^\nu = R[D] + K^2 - K_{ij}K^{ij} = 0 \tag{2.120c}$$

and the momentum constraint

$$\mathbf{M}_i \equiv E_{\mu i}n^\mu = D_i K - D^j K_{ij} = 0. \tag{2.120d}$$

Andersson and Moncrief consider a modified version of the system (2.120) by imposing constant mean curvature (CMC) slicing[5]

[5]We see that the mean curvature K is constant over the slices Σ_t, but not necessarily in time. As it is mentioned in [80], they could also have considered a prescribed mean curvature slicing, i.e. $K = s(t, x)$.

$$K \equiv h^{ij} K_{ij} = t \tag{2.121}$$

and a spatial harmonic (SH) gauge condition

$$V^i \equiv h^{kl} \left(\Gamma^i_{kl} - \tilde{\Gamma}^i_{kl} \right) = 0. \tag{2.122}$$

In this approach there are two sets of evolution equations. The first one is the defining equation of the extrinsic curvature (2.120a), the second is obtained by modifying equation (2.120b) by adding $-D_{(i}V_{j)}$ to the RHS of (2.120b):

$$(\partial_t - \mathcal{L}_\beta) h_{ij} = -2\alpha K_{ij} \tag{2.123a}$$

$$\begin{aligned}(\partial_t - \mathcal{L}_\beta) K_{ij} = -D_i D_j \alpha + \alpha \Big(& R[D]_{ij} - D_{(i}V_{j)} \\ & + K K_{ij} - 2K_{ik} K^k{}_j \Big).\end{aligned} \tag{2.123b}$$

Equations (2.120c) and (2.120d) are replaced by the modified constraints that can be regarded as the equations that determine the lapse function and the shift vector:

$$-D^i D_i \alpha + \alpha K_{ij} K^{ij} = 1 \tag{2.123c}$$

$$\begin{aligned}D^k D_k \beta^i + R[D]^i{}_j \beta^j - \mathcal{L}_\beta V^i = {} & 2D^k \beta^l \left(\Gamma^i_{kl} - \mathring{\Gamma}^i_{kl} \right) \\ & - 2\alpha K^{kl} \left(\Gamma^i_{kl} - \mathring{\Gamma}^i_{kl} \right) + 2K^{ij} D_j \alpha - D^i \alpha K\end{aligned} \tag{2.123d}$$

Equation (2.123c) can be obtained by taking the trace of (2.123b), using the Hamiltonian constraint to trade in the Ricci curvature $R[D]$ for lower order terms and using the CMC condition to set $(\partial_t - \mathcal{L}_\beta) K = 1$.

Equation (2.123d) can be derived as follows. Taking the time derivative of V^i and commuting ∂_t with h^{kl} and the spatial derivatives, one easily obtains

$$\begin{aligned}\partial_t V^i = {} & D^k D_k V^i + R[D]^i{}_j \beta^j + \left(2\alpha K^{kl} - 2D^k \beta^l \right) \left(\Gamma^i_{kl} - \mathring{\Gamma}^i_{kl} \right) \\ & - 2D_j (\alpha K^{ij}) + D^i (\alpha K).\end{aligned} \tag{2.124}$$

Using the momentum constraint, the CMC slicing condition ($D_i K = 0$) and the spatial harmonic condition $(\partial_t - \mathcal{L}_\beta) V^i = 0$ to eliminate second derivatives of the spatial metric and first derivatives of the extrinsic curvature then yields (2.123d). It is worth emphasizing that the CMC slicing condition was used to arrive at both equation (2.123c) and (2.123d).

Now we move on to the question of well-posedness of the system (2.123a-2.123d) in Sobolev spaces and consider initial data $h_{ij}, \alpha, \beta^i \in H^s$ and $K_{ij} \in H^{s-1}$ ($s > \frac{5}{2}$ in 4-dimensional spacetime) that satisfies the Hamiltonian and momentum constraints. For simplicity, we will assume that the spacetime is globally hyperbolic $M = \mathbb{R} \times \Sigma$ where Σ is a compact Riemannian manifold. Similar results can be obtained in the case when Σ is asymptotically Euclidean.

The modified constraints (2.123c,2.123d) are equations relating derivatives of α, β^i up to second order to derivatives of h_{ij} up to first order (including the extrinsic curvature), when written in coordinates. This statement is obvious for (2.123c) but one can check that the second derivatives of h_{ij} cancel each other out on the LHS of (2.123d). More precisely, the modified constraints have the form

$$\mathbf{A}(h, \partial h, K)u = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{2.125}$$

with $u = (\alpha, \beta^i)^T$ and $\mathbf{A}$ is a second order linear elliptic differential operator, with coefficients depending only on the spatial metric, its first spatial derivatives and the extrinsic curvature. Moreover, the elliptic operator $\mathbf{A}$ is lower triangular:

$$\mathbf{A} = \begin{pmatrix} -D^i D_i + K_{ij}K^{ij} & 0 \\ \mathbf{B}^i(h, \partial h, K) & \mathbf{C}^i{}_j(h, \partial h, K) \end{pmatrix} \tag{2.126}$$

with

$$\begin{aligned} \mathbf{C}^i{}_j(h, \partial h, K)\beta^j \equiv & -D^k D_k \beta^i - R[D]^i{}_j \beta^j + \mathcal{L}_\beta V^i \\ & - 2D^k \beta^l \left(\Gamma^i_{kl} - \mathring{\Gamma}^i_{kl}\right). \end{aligned} \tag{2.127}$$

Standard results in the theory of elliptic PDEs (see e.g. Appendix II of [90]) show that the scalar elliptic operator $-D^i D_i + K_{ij}K^{ij}$ is an isomorphism $H^s \to H^{s-2}$ on compact manifolds. Furthermore, it is proved in [80] that the elliptic operator $\mathbf{C}^i{}_j$ is an isomorphism $H^s \to H^{s-2}$, if (Σ, h) is a compact manifold with negative Ricci curvature. These results and the lower triangular structure of $\mathbf{A}$ then implies that $\mathbf{A}$ is also an isomorphism $H^s \to H^{s-2}$. Therefore, if we a priori assume that $h_{ij} \in H^s$ and $K_{ij} \in H^{s-1}$, then the unique solutions α, β^i to the modified constraints are in H^{s+1}, i.e. they have an extra regularity compared to h_{ij}. This is necessary because this way the terms involving first derivatives of β^i in (2.123a) and second derivatives of α in (2.123b) are nonprincipal.

It follows that by solving the modified constraints to determine α and β^i, the evolution equations become a first order quasilinear system of pseudodifferential equations (since the solutions α and β^i have a nonlocal dependence on the spatial metric and the extrinsic curvature). It is easy to see now that the resulting system of evolution equations is strongly hyperbolic, following section 1.2.5[6]. The characteristic equation of the evolution system can be written as

$$\xi_0 \begin{pmatrix} \hat{\gamma}_{ij} \\ 2\hat{\kappa}_{ij} \end{pmatrix} = \mathbb{M}_0(\xi)_{ij}^{kl} \begin{pmatrix} \hat{\gamma}_{kl} \\ 2\hat{\kappa}_{kl} \end{pmatrix} \tag{2.128}$$

where $\mathbb{M}_0$ is the 2×2 block matrix (recall that the terms involving second derivatives of α and first derivatives of β^i are nonprincipal)

$$\mathbb{M}_0(\xi)_{ij}^{kl} = \begin{pmatrix} (\beta^m \xi_m)\, h_i^k h_j^l & -\alpha h_i^k h_j^l \\ -\alpha |\xi|_h^2 h_i^k h_j^l & (\beta^m \xi_m)\, h_i^k h_j^l \end{pmatrix}. \tag{2.129}$$

It is easy to see that $\mathbb{M}_0$ has eigenvalues $\xi_0^{\pm} = \beta^k \xi_k \pm \alpha |\xi|_h$ with a complete set of eigenvectors: for any symmetric matrix u_{ij},

$$\begin{pmatrix} \hat{\gamma}_{ij} \\ 2\hat{\kappa}_{ij} \end{pmatrix} = \begin{pmatrix} u_{ij} \\ \mp (n^\mu \xi_\mu)\, u_{ij} \end{pmatrix} \tag{2.130}$$

is an eigenvector where $\xi_\mu = (\xi_0, \xi_i)$. Note that this means that ξ_μ is null. Since all eigenvalues are real and the eigenvectors can be chosen to be independent of ξ_k, the system of evolution equations is strongly hyperbolic when the modified constraints are solved. (In fact, it is symmetric hyperbolic so one can demonstrate well-posedness by standard energy methods in physical space, as was done in [80].)

[6]A caveat in this argument and the arguments presented in the subsequent sections on cubic Horndeski theories is that in section 1.2.5 we only studied differential systems rather than pseudodifferential systems. However, the original argument of Andersson and Moncrief is rigorous. It seems likely that applying similar estimates to those of [80] in the cubic Horndeski case (or using pseudodifferential calculus to improve the discussion of section 1.2.5) would yield a rigorous proof.

2.A.2 Equations of motion and gauge fixing in cubic Horndeski theories

We will now show that the above formalism can be extended to cubic Horndeski theories. For this, we first discuss the generalization of the SH-CMC gauge condition. Recall that the CMC condition in general relativity was used to set $(\partial_t - \mathcal{L}_\beta)K$ to 1 in the trace of the evolution equation. When taking the trace of (2.9), it is possible to get a constraint equation by a choice of an appropriate slicing condition which sets the terms involving $(\partial_t - \mathcal{L}_\beta)K$ and $(\partial_t - \mathcal{L}_\beta)K_\phi$ to an a priori fixed function. We can proceed similarly for cubic Horndeski theories: in the trace of (2.9) we trade in $R[D]$ using the Hamiltonian constraint to get

$$\begin{aligned} 0 \;=\; & -(\partial_t - \mathcal{L}_\beta)K - \frac{1}{2}\partial_X G_3(12K_\phi^2 - D_k\phi D^k\phi)(\partial_t - \mathcal{L}_\beta)K_\phi \\ & -D^iD_i\alpha - \frac{1}{4}\partial_X G_3\left(12K_\phi^2 - D^k\phi D_k\phi\right)D^i\phi D_i\alpha \\ & +\alpha\Big\{K_{ij}K^{ij} + 2K_\phi^2 + \frac{1}{2}G_2 + \frac{1}{4}\left(4K_\phi^2 + D^k\phi D_k\phi\right)\partial_X G_2 \\ & \quad +4K_\phi^2\partial_\phi G_3 + \partial_X G_3\Big(-4K_\phi D^i\phi D_i K_\phi - 2K_\phi K_{ij}D^i\phi D^j\phi \\ & \quad +\frac{1}{4}\left(4K_\phi^2 + D^k\phi D_k\phi\right)\left(D^iD_i\phi + 2KK_\phi\right)\Big)\Big\} \end{aligned} \tag{2.131}$$

We are seeking a gauge condition of the form

$$K + f(\phi, K_\phi, D_i\phi, h_{kl}) = s(x,t) \tag{2.132}$$

(where s is an arbitrary function) to eliminate the time derivatives in equation (2.131). Taking the normal derivative of (2.132) gives

$$\begin{aligned} (\partial_t - \mathcal{L}_\beta)s(x,t) \;=\; & (\partial_t - \mathcal{L}_\beta)K - 2\alpha\, \partial_\phi f K_\phi + \partial_{K_\phi} f\; (\partial_t - \mathcal{L}_\beta)K_\phi \\ & -2\partial_{D_k\phi} f D_k(\alpha K_\phi) - 2\alpha K_{kl}\frac{\partial f}{\partial h_{kl}}. \end{aligned} \tag{2.133}$$

Therefore, the desired choice is an f satisfying

$$\partial_{K_\phi} f = \frac{1}{2}\partial_X G_3\left(12K_\phi^2 - D_k\phi D^k\phi\right). \tag{2.134}$$

Note that this slicing condition has an interesting relationship with the canonical momentum π^{ij} conjugate to h_{ij}. If we switch to a Hamiltonian description, equation

(2.131) (which is the trace of (2.9)) is equivalent to the trace of

$$\partial_t \pi^{ij} = -\frac{\delta \mathcal{H}}{\delta h_{ij}} \tag{2.135}$$

where $\mathcal{H}$ is the Hamiltonian. Hence, it is clear that the time differentiated terms in (2.131) come from $\partial_t(h_{ij}\pi^{ij})$, that is, the preferred slicing condition is equivalent to $\pi = s(x,t)$.

Rewriting $G_3(\phi, X)$ as a function depending on ϕ, K_ϕ, $D_i\phi$ and h^{ij}, the condition (2.134) can be integrated in K_ϕ and so f can be determined up to the addition of an arbitrary function of ϕ, h_{ij} and $D_i\phi$. Hence, the elliptic equation for α reads as

$$\begin{aligned}
(\partial_t - \mathcal{L}_\beta)s(x,t) \;=\; & -D^iD_i\alpha - \left[\frac{1}{4}\partial_X G_3 \left(12K_\phi^2 - D^k\phi D_k\phi\right) D^i\phi + 2K_\phi \partial_{D_i\phi} f\right] D_i\alpha \\
& +\alpha\Bigg\{ K_{ij}K^{ij} + 2K_\phi^2 - 2\partial_\phi f K_\phi - 2K_{ij}\frac{\partial f}{\partial h_{ij}} - 2\partial_{D_i\phi} f D_i K_\phi \\
& \quad + \frac{1}{2}G_2 + \frac{1}{4}\left(4K_\phi^2 + D^k\phi D_k\phi\right)\partial_X G_2 + 4K_\phi^2 \partial_\phi G_3 \\
& \quad + \partial_X G_3\Big(-4K_\phi D^i\phi D_i K_\phi - 2K_\phi K_{ij} D^i\phi D^j\phi\Big) \\
& \quad + \frac{1}{4}\left(4K_\phi^2 + D^k\phi D_k\phi\right)\left(D^iD_i\phi + 2KK_\phi\right)\Bigg\}.
\end{aligned} \tag{2.136}$$

Regarding the spatial gauge condition, we continue to use the spatial harmonic gauge

$$V^i = 0 \tag{2.137}$$

where V^i is defined in equation (2.122). Once again, we can derive an elliptic equation for the shift vector as in vacuum GR. We require $(\partial_t - \mathcal{L}_\beta)V^i = 0$ and we eliminate derivatives of the extrinsic curvature by using the momentum constraint and the generalized CMC condition. The result is

$$\begin{aligned}
0 \;=\; & D^kD_k\beta^i + R^i_j\beta^j - \mathcal{L}_\beta V^i + 2\left(\alpha K^{kl} - D^k\beta^l\right)\left(\Gamma^i_{kl} - \tilde{\Gamma}^i_{kl}\right) \\
& -2K^{ij}D_j\alpha + KD^i\alpha + \alpha D^i f \\
& +\alpha\Bigg\{ -2K_\phi\Big(1 + \partial_X G_2 + 2\partial_\phi G_3\Big)D^i\phi \\
& \quad + \partial_X G_3\Big(-2K_\phi D^i\phi\left(D^kD_k\phi + 2KK_\phi\right) + K_{kl}D^k\phi D^l\phi D^i\phi \\
& \quad -8K_\phi^2 D^iK_\phi + 2D^i\phi D^k\phi D_k K_\phi + 2K_\phi D^k\phi D_k D^i\phi\Big)\Bigg\}.
\end{aligned} \tag{2.138}$$

Furthermore, using

$$
\begin{aligned}
D^i f &= \partial_\phi f D^i\phi + \partial_{K_\phi} f \; D^i K_\phi + \partial_{D_k\phi} f D^i D_k\phi \\
&= \partial_\phi f D^i\phi + \frac{1}{2}\partial_X G_3 (12K_\phi^2 - D_k\phi D^k\phi)\; D^i K_\phi + \partial_{D_k\phi} f D^i D_k\phi
\end{aligned}
\tag{2.139}
$$

gives

$$
\begin{aligned}
0 \;=\;& D^k D_k \beta^i + R^i_j\beta^j - \mathcal{L}_\beta V^i - \left(-2\alpha K^{kl} + 2D^k\beta^l\right)\left(\Gamma^i_{kl} - \tilde{\Gamma}^i_{kl}\right) \\
& -2K^{ij}D_j\alpha + D^i\alpha K + \alpha\Big\{-2K_\phi\left(1 + \partial_X G_2 + 2\partial_\phi G_3\right) D^i\phi + \partial_\phi f D^i\phi \\
& +\partial_{D_k\phi} f D^i D_k\phi + \partial_X G_3\Big(-2K_\phi D^i\phi\left(D^k D_k\phi + 2KK_\phi\right) + K_{kl}D^k\phi D^l\phi D^i\phi \\
& -\frac{1}{2}\left(4K_\phi^2 + D^k\phi D_k\phi\right) D^i K_\phi + 2D^i\phi D^k\phi D_k K_\phi + 2K_\phi D^k\phi D_k D^i\phi\Big)\Big\}.
\end{aligned}
\tag{2.140}
$$

This is the desired elliptic equation for the shift vector β^i.

To fix the spatial gauge condition, we modify the gravitational evolution equation as before, i.e. we simply replace $\mathcal{E}_{ij}$ by $\tilde{\mathcal{E}}_{ij} \equiv \mathcal{E}_{ij} - D_{(i}V_{j)}$. As mentioned before, we do not modify the scalar equation $\tilde{E}_\phi$ by the gauge-fixing terms. Hence, the scalar evolution equation remains (2.13) and equation (2.9) is replaced by

$$
\begin{aligned}
0 \;=\;& -\left(\partial_t - \mathcal{L}_\beta\right) K_{ij} - \partial_X G_3 (X h_{ij} + D_i\phi D_j\phi)\left(\partial_t - \mathcal{L}_\beta\right) K_\phi \\
& -D_i D_j\alpha + \alpha\Big\{R[D]_{ij} - D_{(i}J_{j)} + KK_{ij} - 2K_{ik}K^k_j \\
& +\frac{1}{2}h_{ij}\left(G_2 - X\partial_X G_2 - X\partial_X G_3\left(D^k D_k\phi - 2K_\phi K + D^k\phi D_k \ln\alpha\right)\right) \\
& -\frac{1}{2}\left(1 + \partial_X G_2 + 2\partial_\phi G_3\right) D_i\phi D_j\phi \\
& +\frac{1}{2}\partial_X G_3\Big(D^k\phi D_k\left(D_i\phi D_j\phi\right) - D_i\phi D_j\phi D^k D_k\phi + 2D_i\phi D_j\phi K_\phi K \\
& -D_i\phi D_j\phi D^k\phi D_k\ln\alpha - 8K_\phi D_{(i}\phi D_{j)}K_\phi\Big)\Big\}.
\end{aligned}
\tag{2.141}
$$

To summarize, the Cauchy problem for cubic Horndeski theories can be formulated as follows. Consider initial data $h_{ij}, \alpha, \beta^i, \phi \in H^s$ and $K_{ij}, K_\phi \in H^{s-1}$ $(s > \frac{9}{2})$[7] that satisfies the Hamiltonian and momentum constraints. Then the system of equations to be solved consists of the evolution equations (2.7), (2.8), (2.13) and (2.141), together with the elliptic equations (2.136), (2.140).

[7]Since the scalar evolution equation (2.13) is not quasilinear, we require more regular initial data than in the case of vacuum GR.

2.A.3 Constraint propagation

In this section we explain how to derive the equations describing the propagation of the gauge conditions and the original constraints from the gauge-fixed equations of motion. As described in the previous section, we use $\tilde{\mathcal{E}}_{ij} \equiv \mathcal{E}_{ij} - D_{(i}V_{j)} = 0$ as the gravitational evolution equation. Following the argument started in section 2.2.2, we set $\tilde{\mathcal{E}}_{ij} = 0$, $\tilde{E}_\phi = 0$ and switch to the new variables

$$\mathbf{F} \equiv K + f - s(x,t), \tag{2.142a}$$

$$\mathbf{V}_i \equiv V_i, \tag{2.142b}$$

$$\tilde{\mathbf{H}} \equiv 2\mathbf{H} - D^k\mathbf{V}_k \tag{2.142c}$$

and

$$\tilde{\mathbf{M}}_i = 2\mathbf{M}_i - D_i\mathbf{F}. \tag{2.142d}$$

We have the following system of homogeneous linear evolution equations

$$\left(\partial_t - \mathcal{L}_\beta\right)\mathbf{F} = \alpha\tilde{\mathbf{H}} \tag{2.143a}$$

$$\left(\partial_t - \mathcal{L}_\beta\right)\mathbf{V}_i = \alpha\tilde{\mathbf{M}}_i \tag{2.143b}$$

$$\begin{aligned}\left(\partial_t - \mathcal{L}_\beta\right)\tilde{\mathbf{H}} = {} & 2\alpha K\tilde{\mathbf{H}} + D^i\alpha\tilde{\mathbf{M}}_i + 2\alpha D_{(i}\mathbf{V}_{j)}K^{ij} \\ & + \mathbf{V}^j D_j\left(\alpha K\right) + \alpha D^i D_i\mathbf{F} + 2D_i\alpha D^i\mathbf{F} \\ & + 2\partial_X G_3 K_\phi\Big(D_i\mathbf{J}_j D^i\phi D^j\phi + 4\tilde{\mathbf{H}}K_\phi^2 \\ & + 8D^i\mathbf{V}_i K_\phi^2 + 2K_\phi\tilde{\mathbf{M}}_i D^i\phi + 2K_\phi D^i\phi D_i\mathbf{F}\Big)\end{aligned} \tag{2.143c}$$

$$\begin{aligned}\left(\partial_t - \mathcal{L}_\beta\right)\tilde{\mathbf{M}}_i = {} & \alpha K\tilde{\mathbf{M}}_i + \alpha K D_i\mathbf{F} + D_i\alpha\tilde{\mathbf{H}} \\ & + 2D^j\alpha D_{(i}\mathbf{V}_{j)} + \alpha\left(D^k D_k\mathbf{J}_i + R_{ij}\mathbf{J}^j\right) \\ & - \partial_X G_3 D_i\phi\Big(D_k\mathbf{V}_j D^k\phi D^j\phi + 4\tilde{\mathbf{H}}K_\phi^2 \\ & + 8D^k\mathbf{V}_k K_\phi^2 + 2K_\phi\tilde{\mathbf{M}}_k D^k\phi + 2K_\phi D^k\phi D_k\mathbf{F}\Big).\end{aligned} \tag{2.143d}$$

The first two equations follow easily by recalling the steps we used to get the elliptic equations (2.123c,2.123d) from the evolution equations and the constraints. To show that the quantities $(\mathbf{F}, \mathbf{J}_i, \tilde{\mathbf{H}}, \tilde{\mathbf{M}}_i)$ remain zero during the evolution, we first note that it follows from equations (2.143a,2.143b) that if $(\mathbf{F}, \mathbf{V}_i, \tilde{\mathbf{H}}, \tilde{\mathbf{M}}_i)$ vanish initially then $\partial_t \mathbf{F} = \partial_t \mathbf{V}_i = 0$ on the initial surface. It turns out that one can obtain a simple energy estimate for the system (2.143) without studying the characteristic equation of the system. Consider the energy [8]

$$E_{\text{constraint}}[\Sigma_t] = \frac{1}{2} \int_{\Sigma_t} \mathrm{d}^3 x \sqrt{h} \Big(|\mathbf{F}|^2 + |D\mathbf{F}|_h^2 + |\mathbf{V}|_h^2 + |D\mathbf{V}|_h^2 + |\tilde{\mathbf{H}}|^2 + |\tilde{\mathbf{M}}|_h^2 \Big). \tag{2.144}$$

Specifically, we want to show that $|\partial_t E_{\text{constraint}}| \leq C E_{\text{constraint}}$ for some constant $C(h, K, \alpha)$. Clearly, the action of ∂_t on the volume form can be bounded by a constant. When the time derivative acts on the gauge and constraint quantities, we use (2.143) to exchange the time derivatives. Since the energy (2.144) is invariant under spatial diffeomorphisms, the terms involving Lie derivatives will vanish.

The nonprincipal terms can be estimated by the energy itself. For example,

$$(\partial_t - \mathcal{L}_\beta)|\mathbf{F}|^2 = 2\alpha \mathbf{F}\tilde{\mathbf{H}} \leq C \left(|\mathbf{F}|^2 + |\tilde{\mathbf{H}}|^2 \right) \tag{2.145}$$

$$\begin{aligned}(\partial_t - \mathcal{L}_\beta)|\mathbf{V}|_h^2 &= 2\alpha h^{ij} \mathbf{V}_i \tilde{\mathbf{M}}_j + 2\alpha K^{ij} \mathbf{V}_i \mathbf{V}_j \\ &\leq C \left(|\mathbf{V}|_h^2 + |\tilde{\mathbf{M}}|_h^2 \right).\end{aligned} \tag{2.146}$$

The potentially problematic (principal) terms are

$$(\partial_t - \mathcal{L}_\beta)|\tilde{\mathbf{H}}|^2 \simeq 2\alpha \tilde{\mathbf{H}} D^i D_i \mathbf{F} \sim -2\alpha D^i \tilde{\mathbf{H}} D_i \mathbf{F} \tag{2.147}$$

$$\begin{aligned}(\partial_t - \mathcal{L}_\beta)|D\mathbf{V}|_h^2 &\simeq 2\alpha D_i \mathbf{V}_j D_k \tilde{\mathbf{M}}_l h^{ik} h^{jl} \\ &\sim -2\alpha D^k D_k \mathbf{V}_j \tilde{\mathbf{M}}_l h^{jl}\end{aligned} \tag{2.148}$$

$$(\partial_t - \mathcal{L}_\beta)|D\mathbf{F}|^2 \simeq 2\alpha D_i \mathbf{F} D^i \tilde{\mathbf{H}} \tag{2.149}$$

$$(\partial_t - \mathcal{L}_\beta)|\tilde{\mathbf{M}}|_h^2 \simeq 2\alpha D^k D_k \mathbf{V}_j \tilde{\mathbf{M}}_l h^{jl} \tag{2.150}$$

[8] The steps of the proof of constraint propagation, as well as the expression for the energy, are the same as in [80] (Lemma 4.1.), since the extra terms entering to the equations due to the presence of a scalar field are nonprincipal. Nevertheless, we provide a sketch of the proof for completeness.

where $\simeq$ denotes equivalence up to principal terms and $\sim$ denotes equivalence of the integrands up to integration by parts. We see that the terms containing higher derivatives cancel each other out, giving us the desired result. Therefore, if $E_{\text{constraint}}$ vanishes initially, then it remains zero during the evolution as well, implying $(\mathbf{F}, \mathbf{V}_i, \tilde{\mathbf{H}}, \tilde{\mathbf{M}}_i) = 0$.

2.A.4 Strong hyperbolicity

In this section we sketch an argument for the local well-posedness of the Cauchy problem for the elliptic-hyperbolic system (2.7), (2.8), (2.13), (2.141), (2.136), (2.140).

We assume that the elliptic system (2.136) and (2.140) has a unique solution for any $(h_{ij}, K_{ij}, \phi, K_\phi)$ satisfying the gauge conditions and constraint equations. Here we argue that this is the case if (i) (Σ, h) is a compact manifold with negative (spatial) Ricci curvature, (ii) the fields are ϕ, $h_{ij} \in H^s$; K_ϕ, $K_{ij} \in H^{s-1}$ and G_2, $\partial_X G_2$, $\partial_\phi G_3$, $\partial_X G_3 \in H^{s-2}$ with $s > 9/2$ and (iii) if the Horndeski terms are small corrections to GR, i.e. in the weakly coupled regime (see equation (2.24)). Note that the requirement of small couplings can be translated to conditions on f:

$$\begin{aligned} &|\partial^l_\phi \partial^k_{K_\phi} f| E^{k+1} \ll 1 && k = 0, 1;\ l = 0, 1 \\ &|\partial^k_{D^i\phi} f| E^{k+1} \ll 1 && k = 0, 1 \\ &|\partial^k_{h_{ij}} f| E^{k+1} \ll 1 && k = 0, 1; \end{aligned} \tag{2.151}$$

with $E = \max\left\{ |R_{\mu\nu\rho\sigma}|^{1/2}, |\nabla_\mu \phi|, |\nabla_\mu \nabla_\nu \phi|^{1/2} \right\}$ in an orthonormal basis.

To see that this is true we simply use the implicit function theorem (Theorem 4.6), the Sobolev multiplication lemma (see e.g. Appendix I of [90]) and the results outlined in section 2.A.1. It is easy to check that the Sobolev multiplication lemma and assumption (ii) above imply that the operators appearing on the RHS of (2.136)-(2.140) are maps $H^s \to H^{s-2}$. Furthermore, at vanishing Horndeski couplings $G_2, G_3 \equiv 0$, the Fréchet derivative of the operator on the RHS of (2.136)-(2.140) with respect to the variables (α, β^i) is exactly the operator $\mathbf{A}$ of (2.126). The results of Andersson and Moncrief reviewed in section 2.A.1 imply that this operator is an isomorphism $H^s \to H^{s-2}$ under assumptions (i) and (ii). Finally, the implicit function theorem tells us that there exists an open set of Horndeski couplings G_2, G_3 in a neighbourhood of $G_2, G_3 \equiv 0$ such that the operator acting on (α, β^i) in (2.136)-(2.140) is also an isomorphism $H^s \to H^{s-2}$. This concludes the argument on existence and uniqueness of solutions to the elliptic system (2.136)-(2.140).

The discussion of the evolution equations is more cumbersome in cubic Horndeski theories than in GR. The source of the difficulty is that in the elliptic equations (2.136) and (2.140) we could not get rid of the second derivatives of the scalar field and hence the lapse and the shift does not enjoy extra regularity compared to h_{ij} as in GR. This implies that the first derivatives of β^i appearing in the defining equation of the extrinsic curvature (2.7) and the second derivatives of α appearing in the tensor evolution equation (2.141) are now principal terms.

To illustrate how these terms affect the principal symbol, we transform the equations to a more familiar form. Let us act on the evolution equations (2.7), (2.8), (2.13), (2.141) with the "Laplacian" operator $\Delta \equiv h^{kl}\mathring{D}_k\mathring{D}_l$ and let us introduce the variables.

$$(\gamma_{ij}, \kappa_{ij}, \psi, k, a, b^i) \equiv (\Delta h_{ij}, \Delta K_{ij}, \Delta\phi, \Delta K_\phi, \Delta\alpha, \Delta\beta^i). \tag{2.152}$$

In the new evolution equations the derivatives of a and b^i can be converted to derivatives of the scalar field by using the derivatives of the elliptic equations (2.136), (2.140):

$$\begin{aligned} \partial_m a \quad &\simeq \quad \frac{1}{4}\alpha\partial_X G_3 \left(4K_\phi^2 + D^k\phi D_k\phi\right)\partial_m\left(h^{ij}\partial_i\partial_j\phi\right) \\ &\quad +2\alpha\left(-\partial_{D_k\phi}f - 2\partial_X G_3 K_\phi D^i\phi\right)\partial_m(\partial_i K_\phi) \end{aligned} \tag{2.153}$$

$$\begin{aligned} \partial_m b^i \quad &\simeq \quad -2\alpha\left[\partial_X G_3 D^i\phi D^j\phi - \frac{1}{4}\partial_X G_3\left(4K_\phi^2 + D^k\phi D_k\phi\right)h^{ij}\right]\partial_m(\partial_j K_\phi) \\ &\quad -\alpha\left[\left(\partial_{D_k\phi}f + 2\partial_X G_3 K_\phi D^k\phi\right)h^{il} - 2\partial_X G_3 K_\phi D^i\phi h^{kl}\right]\partial_m(\partial_k\partial_l\phi) \end{aligned} \tag{2.154}$$

In the resulting system the principal terms will have the same form as in (1.75)-(1.76) and thus we can study its characteristic equation using methods presented in section 1.2.5. Let us denote the components of the polarization vector U (which is a 14-component column vector in this case) by

$$U = \left[\hat{\gamma}_{ij}, \hat{\kappa}_{ij}, \hat{\psi}, \hat{a}\right]^T.$$

Then the rows of the characteristic equation can be written as follows.

$$\frac{1}{\alpha}\left(\xi_0 - \beta^k\xi_k\right)\hat{\gamma}_{ij} = -2\hat{\kappa}_{ij} + \frac{2}{\alpha}h_{l(i}\xi_{j)}b^l(\xi), \tag{2.155a}$$

$$\frac{1}{\alpha}\left(\xi_0-\beta^k\xi_k\right)\hat{\psi}=-2\hat{k}, \tag{2.155b}$$

$$\begin{aligned}\frac{1}{\alpha}\left(\xi_0-\beta^k\xi_k\right)\ 2\hat{\kappa}_{ij} \quad = \quad & -\frac{2}{\alpha}\partial_X G_3\left(Xh_{ij}+D_i\phi D_j\phi\right)\left(\xi_0-\beta^k\xi_k\right)\hat{k} \\ & -|\xi|_h^2\hat{\gamma}_{ij}-\frac{2}{\alpha}\xi_i\xi_j\hat{a}(\xi) \\ & -\partial_X G_3\Big((Xh_{ij}+D_i\phi D_j\phi)|\xi|_h^2\hat{\psi} \\ & -D^k\phi\ \xi_k D_{(i}\phi\ \xi_{j)}\hat{\psi}-8K_\phi D_{(i}\phi\ \xi_{j)}\hat{k}\Big),\end{aligned} \tag{2.155c}$$

$$\mathcal{A}\frac{1}{\alpha}\left(\xi_0-\beta^k\xi_k\right)\hat{a}=\mathcal{B}(\xi)\hat{k}+\mathcal{C}(\xi)\hat{\psi} \tag{2.155d}$$

where the specific expressions for the functions $\mathcal{A}$, $\mathcal{B}$ and $\mathcal{C}$ are quite long and unessential for our purposes (although they can be straightforwardly computed from (2.13)), and the expressions for $\hat{a}$, $\hat{b}^i$ are given by[9]

$$\begin{aligned}\hat{a}(\xi) \quad = \quad & \frac{1}{4}\alpha\partial_X G_3\left(4K_\phi^2+D^k\phi D_k\phi\right)\hat{\psi} \\ & +2\alpha\left(-\partial_{D_k\phi}f-2\partial_X G_3 K_\phi D^k\phi\right)\frac{\xi_k}{|\xi|_h^2}\hat{k}\end{aligned} \tag{2.156}$$

$$\begin{aligned}\hat{b}^i(\xi) \quad = \quad & -2\alpha\left[\partial_X G_3 D^i\phi D^j\phi-\frac{1}{4}\partial_X G_3\left(4K_\phi^2+D^k\phi D_k\phi\right)h^{ij}\right]\frac{\xi_j}{|\xi|_h^2}\hat{k} \\ & +\alpha\left[\left(-\partial_{D_k\phi}f-2\partial_X G_3 K_\phi D^k\phi\right)\frac{\xi^i\xi_k}{|\xi|_h^2}+2\partial_X G_3 K_\phi D^i\phi\right]\hat{\psi}.\end{aligned} \tag{2.157}$$

The only property of the functions $\mathcal{A}$, $\mathcal{B}$ and $\mathcal{C}$ that we need to use is that substituting (2.155b) into (2.155d) gives (recall equation (2.21))

$$\hat{\psi}\left(P'_{\phi\phi}\right)^{\mu\nu}\xi_\mu\xi_\nu=0. \tag{2.158}$$

Now we are ready to discuss the eigenvalues and eigenvectors solving the characteristic equations (2.155a)-(2.155d). It follows from the upper triangular structure of the

[9]Solving the elliptic equations (2.136)-(2.140) for α, β^i and with fixed ϕ, K_ϕ, h_{ij}, K_{ij}, one obtains a (nonlocal) map $(\alpha,\beta):(\phi,K_\phi,h_{ij},K_{ij})\to(\alpha,\beta)$. This solution map is a pseudodifferential operator of class $\mathcal{OP}^{-2}_{\rm cl}$ whose principal symbol is given by (2.156), (2.157) (see e.g. [41,91]).

characteristic equation (see Section 2.2) that

$$\left[\hat{\gamma}_{ij}, \hat{\kappa}_{ij}, \hat{\psi}, \hat{k}\right]^T = \left[\hat{u}_{ij}, -\frac{1}{2}\left(n^\mu \xi^\pm_\mu\right)\hat{u}_{ij}, 0, 0\right]^T \tag{2.159}$$

is an eigenvector of (2.155a-2.155d) with eigenvalues $\xi_0^\pm = \beta^k\xi_k \pm \alpha|\xi|_h$ for any symmetric $\hat{u}_{ij}$. (Recall that $\xi_\mu = (\beta^k\xi_k \pm \alpha|\xi|_h, \xi_i)$ is a null vector with respect to the spacetime metric.) One can easily find 6 linearly independent vectors $\hat{u}_{ij}$. Taking into account the two sign choices in $\xi_0^\pm$ and in (2.159), this gives 12 eigenvectors: a 6-dimensional degenerate eigenspace for both eigenvalues $\xi_0^\pm = \beta^k\xi_k \pm \alpha|\xi|_h$.

The remaining eigenvalues $\xi_0^{\phi,\pm}$ are found by solving

$$\left(P'_{\phi\phi}\right)^{\mu\nu}\xi_\mu\xi_\nu = 0 \tag{2.160}$$

(see Section 2.2 for notation). Recall that for small couplings, $\xi_0^{\phi,\pm}$ are distinct, nonzero and real. The corresponding eigenvectors have the form

$$\left[\hat{\gamma}_{ij}, \hat{\kappa}_{ij}, \hat{\psi}, \hat{a}\right]^T = \left[\hat{\gamma}^\phi_{ij}, \hat{\kappa}^\phi_{ij}, 1, -\frac{1}{2}\left(n^\mu\xi_\mu\right)\right]^T \tag{2.161}$$

with

$$\begin{aligned}\hat{\gamma}^\phi_{ij} &= -\partial_X G_3\left(Xh_{ij} + D_i\phi D_j\phi\right) + \frac{2}{|\xi|_h^2}\partial_X G_3 \xi_k D^k\phi D_{(i}\phi\ \xi_{j)} \\ &\quad -\frac{\xi_i\xi_j}{2|\xi|^2_h}\partial_X G_3\left(4K_\phi^2 + D^k\phi D_k\phi\right)\end{aligned} \tag{2.162}$$

$$\begin{aligned}2\hat{\kappa}^\phi_{ij} &= \left(n^\mu\xi^{\phi,\pm}_\mu\right)\partial_X G_3\left(Xh_{ij} + D_i\phi D_j\phi\right) \\ &\quad +2\left[\left(-\partial_{D_k\phi}f - 2\partial_X G_3 K_\phi D^k\phi\right)\frac{\xi_i\xi_j\xi_k}{|\xi|^2_h} + 2\partial_X G_3 K_\phi D_{(i}\phi\ \xi_{j)}\right].\end{aligned} \tag{2.163}$$

These expressions are clearly smooth functions of ξ_i since h_{ij} is a positive definite metric and $\xi_i \neq 0$ by assumption (ξ_i has unit norm).

We can identify 3 pairs of eigenmodes that are associated with the physical degrees of freedom. There are 2 pairs of transverse-traceless modes whose characteristic covectors are null w.r.t g, i.e.

$$\left[\hat{\gamma}_{ij}, \hat{\kappa}_{ij}, \hat{\psi}, \hat{a}\right]^T = \left[\hat{u}^{TT}_{ij}, -\frac{1}{2}\left(n^\mu\xi^\pm_\mu\right)\hat{u}^{TT}_{ij}, 0, 0\right]^T \tag{2.164}$$

with $\hat{u}^{TT}_{ij}$ satisfying $h^{ij}\hat{u}^{TT}_{ij} = 0$ and $\xi^i \hat{u}^{TT}_{ij} = 0$. These correspond to the two gravitational degrees of freedom that propagate with the speed of light. The eigenvectors corresponding to the scalar degree of freedom are given by (2.161)-(2.163) and their characteristic covectors are null w.r.t. $P'_{\phi\phi}$.

These "physical" eigenvectors satisfy the high frequency limit of the Hamiltonian and momentum constraints

$$2\hat{\mathbf{H}} \equiv \; -2\xi^2 h^{ij}\hat{\gamma}_{ij} + 2\xi^i\xi^j\hat{\gamma}_{ij} + \partial_X G_3 \left(4K_\phi^2 |\xi|_h^2 - (D^k\phi\; \xi_k)^2\right)\hat{\psi} = 0,$$

$$\hat{\mathbf{M}}_i \equiv \xi_i\hat{\kappa} - \xi^j\hat{\kappa}_{ij} - \partial_X G_3\Big(K_\phi D_i\phi |\xi|_h^2 \hat{\psi} - \xi_j\xi_i K_\phi D^j\phi\hat{\psi} + D_i\phi D^k\phi\xi_k\hat{k} - 4\xi_i K_\phi^2\hat{k}\Big) = 0$$

and the high frequency versions of gauge conditions

$$\begin{aligned}
\hat{\mathbf{V}}_i &\equiv \xi^j\hat{\gamma}_{ij} - \frac{1}{2}\xi_i h^{kl}\hat{\gamma}_{kl} = 0\\
\hat{\mathbf{F}} &\equiv h^{ij}\hat{\kappa}_{ij} + \partial_{K_\phi} f\hat{k} + \partial_{D_k\phi} f\xi_k\hat{\psi} = 0
\end{aligned}$$

To summarize, we have found that the characteristic equation (see equations (2.155a-2.155d)) has real eigenvalues and the corresponding eigenvectors are linearly independent and have smooth dependence on ξ_i. This implies that the evolution equations are strongly hyperbolic when the modified constraint equations have a unique solution for arbitrary (ϕ, K_ϕ, h, K). In particular, this is the case in spacetimes that can be foliated with compact slices with generalized prescribed mean curvature and negative (spatial) Ricci curvature.

Chapter 3

Well-posed formulation of Horndeski and Lovelock theories

In this chapter we show that the initial value problem for any weakly coupled Lovelock and Horndeski theories is locally well-posed. The contents of this chapter are the results of original research done in collaboration with Harvey Reall and published in [44]. A short summary of the same results have been published in [68].

3.1 Introduction

To demonstrate that the initial value problem in Lovelock and Horndeski theories is well-posed, we use the methods presented in section 1.2.1 and introduce a formulation of the theories that is strongly hyperbolic at weak coupling.

As mentioned earlier, the original harmonic gauge fixing procedure does not give rise to strongly hyperbolic equations in a general Lovelock or Horndeski theory due to the high degree of degeneracy between different types of mode solutions [60, 61]. The approaches discussed in the previous chapter for cubic Horndeski theories provide only a partial resolution of this issue. For example, in the BSSN formulation (section 2.3) there is a degenerate eigenspace of zero speed modes that contain both pure gauge and constraint-violating modes. This degeneracy cannot be removed with any the choice of the free "gauge source" functions (i.e. the function F in (2.60) and the functions σ, f in (2.109a)-(2.109b)). Therefore, it seems that the three formulations presented in the previous chapter do not give rise to strongly hyperbolic equations in more general Horndeski (and Lovelock) theories.

The approach discussed in this chapter overcomes this problem by introducing a modification of the usual harmonic gauge condition such that the pure gauge modes propagate along the null cone of an auxiliary (inverse) metric $\tilde{g}^{\mu\nu}$ (instead of the null cone of the physical metric as in the original harmonic gauge). We implement this gauge condition by adding a gauge-fixing term to the equation of motion for the physical metric. In this gauge-fixing term we introduce another auxiliary (inverse) metric $\hat{g}^{\mu\nu}$. The effect of this is to obtain a new formulation of GR in which the pure gauge modes propagate along the null cone of $\tilde{g}^{\mu\nu}$, the gauge-condition violating modes propagate along the null cone of $\hat{g}^{\mu\nu}$ and the physical modes propagate along the null cone of $g^{\mu\nu}$. By choosing $\tilde{g}^{\mu\nu}$ and $\hat{g}^{\mu\nu}$ such that these three null cones don't intersect, we ensure that the three different types of mode propagate with different speeds. We will show that this formulation of GR is strongly hyperbolic. Furthermore, the degeneracy discussed above is now absent and so, when we introduce a deformation by turning on Lovelock or Horndeski terms, the theory remains strongly hyperbolic at weak coupling.

The chapter is organized as follows. In section 3.2 we introduce our modified harmonic gauge formulation of vacuum GR and explain why it admits a well-posed initial value problem. In sections 3.3 and 3.4 we extend this formulation to weakly coupled Lovelock and Horndeski theories respectively. Section 3.5 contains further discussion, including the implementation of our formulation in numerical relativity. The focus of this thesis is on gravitational theories but in Appendix 3.A we show that our formulation can also be applied to electromagnetism.

3.2 General relativity in modified harmonic gauge

3.2.1 The modified harmonic gauge equation of motion

Let $g_{\mu\nu}$ be the physical metric. The vacuum Einstein equation is

$$E^{\mu\nu} = 0 \tag{3.1}$$

where

$$E^{\mu\nu} \equiv R^{\mu\nu} - \frac{1}{2}Rg^{\mu\nu} + \Lambda g^{\mu\nu} \tag{3.2}$$

We introduce an auxiliary (inverse) Lorentzian metric $\tilde{g}^{\mu\nu}$ and define

$$H^{\mu} \equiv \tilde{g}^{\rho\sigma}\nabla_{\rho}\nabla_{\sigma}x^{\mu} = -\tilde{g}^{\rho\sigma}\Gamma^{\mu}_{\rho\sigma} \tag{3.3}$$

where quantities without tildes are calculated using the metric $g_{\mu\nu}$ (so H^μ involves both $g_{\mu\nu}$ and $\tilde{g}^{\mu\nu}$). Our modified harmonic gauge condition is

$$H^\mu = 0 \tag{3.4}$$

This is a linear wave equation for x^μ, which admits a well-posed initial value problem for initial data prescribed on a surface Σ that is spacelike w.r.t. $\tilde{g}^{\mu\nu}$. So, at least locally, coordinates can be chosen to satisfy this gauge condition, just as for conventional harmonic gauge [38].

Now introduce another auxiliary (inverse) Lorentzian metric $\hat{g}^{\mu\nu}$ and define

$$E^{\mu\nu}_{\text{mhg}} = E^{\mu\nu} + \hat{P}_\alpha{}^{\beta\mu\nu}\partial_\beta H^\alpha \tag{3.5}$$

where

$$\hat{P}_\alpha{}^{\beta\mu\nu} = \delta_\alpha^{(\mu}\hat{g}^{\nu)\beta} - \frac{1}{2}\delta_\alpha^\beta\hat{g}^{\mu\nu} \tag{3.6}$$

Our modified harmonic gauge equation of motion is

$$E^{\mu\nu}_{\text{mhg}} = 0 \tag{3.7}$$

We have three inverse metrics $g^{\mu\nu}$, $\tilde{g}^{\mu\nu}$ and $\hat{g}^{\mu\nu}$. The inverse of $g^{\mu\nu}$ is denoted, as usual, by $g_{\mu\nu}$ and index raising and lowering is always performed with g. When we need to refer to the inverse of $\hat{g}^{\mu\nu}$ (say) we will write $(\hat{g}^{-1})_{\mu\nu}$. The usual harmonic gauge formulation of GR is obtained by choosing $\hat{g}^{\mu\nu} = \tilde{g}^{\mu\nu} = g^{\mu\nu}$.

We will assume that $\hat{g}^{\mu\nu}$ is chosen so that the causal cone of $g^{\mu\nu}$ (in the cotangent space) lies strictly inside the causal cone of $\hat{g}^{\mu\nu}$, so that any covector that is causal w.r.t. $g^{\mu\nu}$ is timelike w.r.t. $\hat{g}^{\mu\nu}$. See Fig. 3.1a. This implies that the causal cone of $(\hat{g}^{-1})_{\mu\nu}$ (in the tangent space) lies strictly inside the causal cone of $g_{\mu\nu}$ (Fig. 3.1b) so any smooth curve that is causal w.r.t. $(\hat{g}^{-1})_{\mu\nu}$ is timelike w.r.t. $g_{\mu\nu}$. This implies that any point in the domain of dependence $D(\Sigma)$ of a partial Cauchy surface Σ w.r.t. $g_{\mu\nu}$ is also in the domain of dependence $\hat{D}(\Sigma)$ of Σ w.r.t. $(\hat{g}^{-1})_{\mu\nu}$. In other words, $D(\Sigma) \subset \hat{D}(\Sigma)$.

We will also assume that $\tilde{g}^{\mu\nu}$ is chosen so that the causal cones of the three inverse metrics form a nested set as in Fig. 3.1a, with the null cones of $\hat{g}^{\mu\nu}$ and $\tilde{g}^{\mu\nu}$ lying outside the null cone of $g^{\mu\nu}$. This implies that a surface Σ that is spacelike w.r.t. $g^{\mu\nu}$ is also spacelike w.r.t. $\hat{g}^{\mu\nu}$ and $\tilde{g}^{\mu\nu}$.

In Fig 3.1 we have drawn the null cone of $\tilde{g}^{\mu\nu}$ inside that of $\hat{g}^{\mu\nu}$ but we could also choose it to lie outside. What is important is that these null cones do not intersect and that they both lie outside that of $g^{\mu\nu}$.[1]

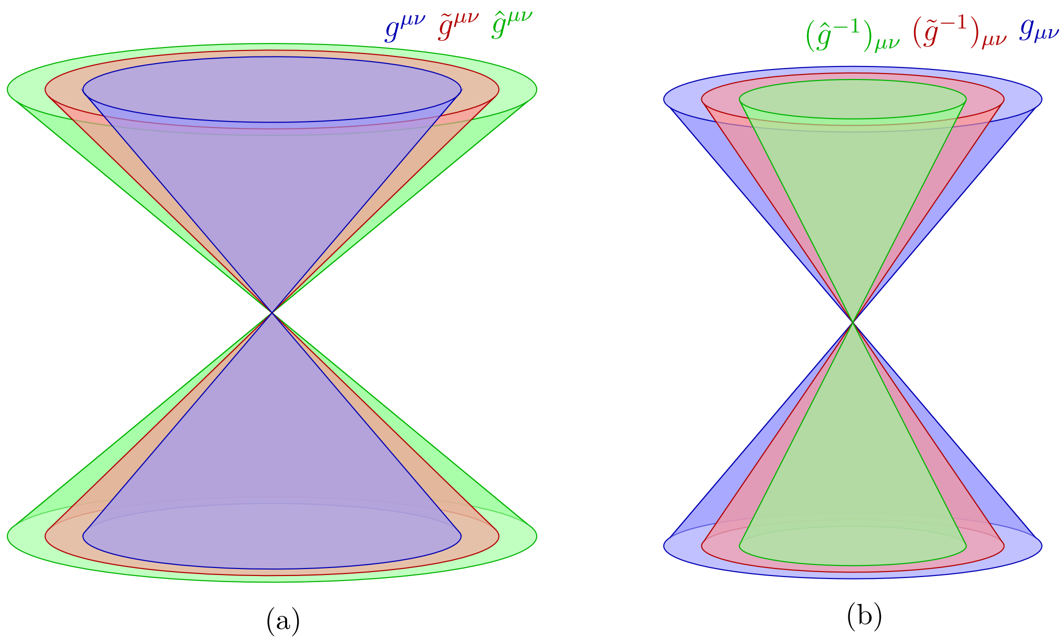

Fig. 3.1 (a) Cotangent space at a point, showing the null cones of $g^{\mu\nu}$, $\tilde{g}^{\mu\nu}$ and $\hat{g}^{\mu\nu}$. (b) Tangent space at a point, showing the null cones of $g_{\mu\nu}$, $(\tilde{g}^{-1})_{\mu\nu}$ and $(\hat{g}^{-1})_{\mu\nu}$.

Since the causal cones of the three metrics form a nested set, there are no subtleties with defining time orientations for the unphysical auxiliary metrics. Given a time orientation for the physical metric $g_{\mu\nu}$ we define the future (past) causal cone of $(\hat{g}^{-1})_{\mu\nu}$ to be the one inside the future (past) causal cone of $g_{\mu\nu}$ and similarly for $(\tilde{g}^{-1})_{\mu\nu}$.

In Appendix 3.A we explain how our modified harmonic gauge condition and gauge-fixing procedure can also be applied to Maxwell theory, which gives a "modified Lorenz gauge" formulation of Maxwell's equations.

3.2.2 Propagation of the gauge condition

Our first task is to show that solutions of (3.7) are also solutions of the vacuum Einstein equation provided that the initial data satisfies the constraint equations and the modified harmonic gauge condition. The argument follows closely the usual

[1] In section 3.5 we will comment on how the latter assumption might be relaxed in numerical relativity applications.

argument for harmonic gauge GR [38]. Given a solution $g_{\mu\nu}$ of (3.7) on a manifold M, the contracted Bianchi identity gives

$$0 = \nabla_\nu E^{\mu\nu}_{\text{mhg}} = \frac{1}{2}\hat{g}^{\alpha\beta}\partial_\alpha\partial_\beta H^\mu + \dots \tag{3.8}$$

where the ellipsis denotes terms linear in first derivatives of H^ρ. Thus the modified harmonic gauge equation of motion implies that H^μ satisfies a linear wave equation with principal symbol $(1/2)\hat{g}^{\alpha\beta}\xi_\alpha\xi_\beta$. Let $\Sigma \subset M$ be a surface that is spacelike with future-directed unit normal n^μ w.r.t. $g^{\mu\nu}$. Then Σ is also spacelike w.r.t. $\hat{g}^{\mu\nu}$ so (3.8) admits a well-posed initial value problem for initial data H^μ and $\hat{g}^{\nu\rho}n_\nu\partial_\rho H^\mu$ prescribed on Σ. If H^μ and $\hat{g}^{\nu\rho}n_\nu\partial_\rho H^\mu$ vanish on Σ then it follows from well-posedness of the initial value problem for (3.8) that H^μ vanishes throughout the domain of dependence $\hat{D}(\Sigma) \subset M$. Hence (M, g) will satisfy the vacuum Einstein equation $E^{\mu\nu} = 0$ in $\hat{D}(\Sigma)$. Since $D(\Sigma) \subset \hat{D}(\Sigma)$, it then follows that (M, g) satisfies the Einstein equation in $D(\Sigma)$.

Now consider the initial value problem for (3.7). In GR, initial data is a triple (Σ, h_{ij}, K_{ij}) where Σ is a 3-manifold and, in some chart x^i on Σ, h_{ij} and K_{ij} are the components of a Riemannian metric and a symmetric tensor on Σ. These must satisfy the usual constraint equations of GR. We now parameterize the metric $g_{\mu\nu}$ in terms of a lapse function and shift vector in the usual way, which ensures that surfaces of constant x^0 are spacelike w.r.t. $g_{\mu\nu}$ and hence also w.r.t. $\hat{g}^{\mu\nu}$ and $\tilde{g}^{\mu\nu}$. At $x^0 = 0$ the lapse and shift can be chosen arbitrarily. Given a choice of lapse and shift, the values of g_{ij} and $\partial_0 g_{ij}$ at $x^0 = 0$ are fixed by requiring that the surface $x^0 = 0$ matches the data on Σ, i.e., it has induced metric h_{ij} and extrinsic curvature K_{ij}.

The time derivatives of the lapse and shift at $x^0 = 0$ are fixed by requiring that $H^\mu = 0$ at $x^0 = 0$. This is possible because the equation $H_i = 0$ has the form $\tilde{g}^{00}\partial_0 g_{0i} = \dots$ where the ellipsis denotes terms not involving $\partial_0 g_{0\mu}$. The surface $x^0 = 0$ is spacelike w.r.t. $\tilde{g}^{\mu\nu}$ so $\tilde{g}^{00} \neq 0$ hence $\partial_0 g_{0i}$ can be chosen to ensure that $H_i = 0$. The equation $H_0 = 0$ then has the form $\tilde{g}^{00}\partial_0 g_{00} = \dots$ where the ellipsis is independent of $\partial_0 g_{00}$. Hence $\partial_0 g_{00}$ can be chosen to ensure that $H_0 = 0$.

We have specified initial data $(g_{\mu\nu}, \partial_0 g_{\mu\nu})$ at $x^0 = 0$ that matches the initial data on Σ and satisfies $H^\mu = 0$ at $x^0 = 0$. We can now identify Σ with the surface $x^0 = 0$.

The initial data satisfies the constraint equations of GR so $E^{\mu 0} = 0$ at $x^0 = 0$. Evaluating the 0μ components of (3.7) at $x^0 = 0$ and using the vanishing of the tangential derivative $\partial_i H^\mu$ at $x^0 = 0$, we obtain $\partial_0 H^\mu = 0$ at $x^0 = 0$. Hence all first derivatives of H^μ vanish at $x^0 = 0$ so $\hat{g}^{\nu\rho}n_\nu\partial_\rho H^\mu = 0$ on Σ.

In summary, we have shown that we can choose the initial time derivative of the lapse and shift such that $H^\mu = \hat{g}^{\nu\rho} n_\nu \partial_\rho H^\mu = 0$ on Σ. Hence, if (M, g) is a solution of (3.7) that matches our initial data $(g_{\mu\nu}, \partial_0 g_{\mu\nu})$ on Σ, then $g_{\mu\nu}$ will then satisfy the vacuum Einstein equation throughout $D(\Sigma) \subset M$.

For technical reasons we will explain later, we will demand that the initial lapse and shift are chosen so that $\partial/\partial x^0$ is timelike w.r.t. all three metrics (although this condition may not be necessary for well-posedness). If this condition is satisfied initially then, by continuity, it will hold in a neighbourhood of the initial surface.

3.2.3 Strong hyperbolicity

In this section we will show that the modified harmonic gauge equation of motion (3.7) admits a well-posed initial value problem by demonstrating that (3.7) is strongly hyperbolic. Recall (see section 1.2) that in a second order system of PDEs strong hyperbolicity is a property of the 2nd derivative terms in the equation of motion, i.e., of the principal symbol.

Let ξ_μ be an arbitrary covector. The principal symbol of (3.7), acting on a symmetric tensor $t_{\mu\nu}$, is defined by the replacement $\partial_\mu \partial_\nu g_{\rho\sigma} \to \xi_\mu \xi_\nu t_{\rho\sigma}$ in the terms involving 2nd derivatives. The result is

$$\mathcal{P}(\xi)^{\mu\nu\rho\sigma} t_{\rho\sigma} = \mathcal{P}_\star(\xi)^{\mu\nu\rho\sigma} t_{\rho\sigma} + \mathcal{P}_{\rm GF}(\xi)^{\mu\nu\rho\sigma} t_{\rho\sigma} \tag{3.9}$$

where we have decomposed the RHS into a part arising from the Einstein tensor and a part arising from the gauge-fixing term in (3.7). The part arising from the Einstein tensor is

$$\mathcal{P}_\star(\xi)^{\mu\nu\rho\sigma} t_{\rho\sigma} = -\frac{1}{2} g^{\gamma\delta} \xi_\gamma \xi_\delta P^{\mu\nu\rho\sigma} t_{\rho\sigma} + P_\alpha{}^{\gamma\mu\nu} \xi_\gamma g^{\alpha\beta} P_\beta{}^{\delta\rho\sigma} \xi_\delta t_{\rho\sigma} \tag{3.10}$$

and the part arising from the gauge-fixing term is

$$\mathcal{P}_{\rm GF}(\xi)^{\mu\nu\rho\sigma} t_{\rho\sigma} = -\hat{P}_\alpha{}^{\gamma\mu\nu} \xi_\gamma g^{\alpha\beta} \tilde{P}_\beta{}^{\delta\rho\sigma} \xi_\delta t_{\rho\sigma} \tag{3.11}$$

where we have defined, in analogy with (3.6),

$$P_\alpha{}^{\beta\mu\nu} = \delta_\alpha^{(\mu} g^{\nu)\beta} - \frac{1}{2} \delta_\alpha^\beta g^{\mu\nu} \qquad \tilde{P}_\alpha{}^{\beta\mu\nu} = \delta_\alpha^{(\mu} \tilde{g}^{\nu)\beta} - \frac{1}{2} \delta_\alpha^\beta \tilde{g}^{\mu\nu} \tag{3.12}$$

In conventional harmonic gauge ($\hat{g}^{\mu\nu} = \tilde{g}^{\mu\nu} = g^{\mu\nu}$), the gauge fixing term cancels the second term of (3.10) but this is no longer the case in our modified harmonic gauge.

We will use indices $I, J, \ldots$ to refer to a basis for symmetric tensors, i.e., we will sometimes write t_I instead of $t_{\mu\nu}$. Such indices take values from 1 to $N = d(d+1)/2$, where d is the spacetime dimension. We can then view $\mathcal{P}(\xi)$ as a $N \times N$ matrix $P(\xi)^{IJ}$. If we do this then the matrix $\mathcal{P}_\star(\xi)^{IJ}$ is *symmetric*. Since $\mathcal{P}(\xi)$ is quadratic in ξ_μ we have

$$\mathcal{P}(\xi)^{IJ} = \mathcal{P}^{IJ\gamma\delta}\xi_\gamma\xi_\delta \tag{3.13}$$

where $\mathcal{P}^{IJ\gamma\delta}$ can be read off from the above expressions. In coordinates $x^\mu = (x^0, x^i)$ we can write

$$\mathcal{P}(\xi)^{IJ} = \xi_0^2 A^{IJ} + \xi_0 B^{IJ} + C^{IJ} \tag{3.14}$$

where

$$A^{IJ} = \mathcal{P}^{IJ00} \qquad B^{IJ} = 2\xi_i\mathcal{P}^{IJ0i} \qquad C^{IJ} = \xi_i\xi_j\mathcal{P}^{IJij} \tag{3.15}$$

Note that ξ_i are the components of the pull-back of ξ_μ to the surfaces of constant x^0.

We can write $A^{IJ} = A_\star^{IJ} + A_{\mathrm{GF}}^{IJ}$ etc, and the quantities with a star subscript are symmetric matrices. As explained in section 3.2.2, we can arrange that surfaces of constant x^0 are spacelike w.r.t. $g^{\mu\nu}$, at least in a neighbourhood of our initial value surface. This implies that these surfaces are also spacelike w.r.t. $\hat{g}^{\mu\nu}$ and $\tilde{g}^{\mu\nu}$. We will show below that a covector is characteristic if, and only if, it is null w.r.t. one of these three inverse metrics. Since dx^0 is timelike w.r.t. $g^{\mu\nu}$, it is timelike w.r.t. all three inverse metrics. It follows that dx^0 is non-characteristic, which implies that surfaces of constant x^0 are non-characteristic and hence the matrix A^{IJ} is invertible.

As reviewed in section 1.2, to define strong hyperbolicity we introduce a $(2N) \times (2N)$ real matrix depending on the (real) spatial components ξ_i of ξ_μ (as well as the spacetime coordinates x^μ but we suppress this dependence):

$$M(\xi_i) = \begin{pmatrix} 0 & I \\ -A^{-1}C(\xi_i) & -A^{-1}B(\xi_i) \end{pmatrix} \tag{3.16}$$

We assume there exists a smooth Riemannian inverse metric G^{ij} on surfaces of constant x^0. For example, our condition that $\partial/\partial x^0$ is timelike implies that g^{ij} is positive definite so we could choose $G^{ij} = g^{ij}$. We say that ξ_i is a unit covector if $G^{ij}\xi_i\xi_j = 1$.

Recall that strong hyperbolicity is the statement that, for any (real) unit covector ξ_i, the matrix $M(\xi_i)$ admits a positive definite Hermitian symmetrizer, i.e. a matrix $K(\xi_i)$ that satisfies

$$K(\xi_i)M(\xi_i) = M(\xi_i)^\dagger K(\xi_i). \tag{3.17}$$

The symmetrizer must also satisfy the condition that it depends smoothly on ξ_i and on the spacetime coordinates x^μ that we have suppressed above. Strong hyperbolicity implies that $M(\xi_i)$ is diagonalizable with real eigenvalues. Conversely, if $M(\xi_i)$ is diagonalizable with real eigenvalues then one can construct a symmetrizer provided the eigenvectors of $M(\xi_i)$ depend smoothly on the unit vector ξ_i.

In the argument relating strong hyperbolicity to well-posedness presented in section 1.2 we assumed $\det M \neq 0$ (which is equivalent to $\det C \neq 0$, which is equivalent to the condition that a covector of the form $(0, \xi_i)$ is never characteristic). This is guaranteed by our condition that $\partial/\partial x^0$ is timelike w.r.t. all three metrics, since this implies $\xi_0 \neq 0$ for any covector ξ_μ that is null w.r.t. one of the three metrics, as we will show is the case for a characteristic covector.

We will now determine the eigenvalues and eigenvectors of $M(\xi_i)$. If ξ_0 is an eigenvalue of $M(\xi_i)$ then the eigenvalue equation reduces to the condition that the eigenvector is of the form $(t_I, \xi_0 t_I)^T$ where

$$\mathcal{P}(\xi)^{\mu\nu\rho\sigma} t_{\rho\sigma} = 0 \tag{3.18}$$

with $\xi_\mu = (\xi_0, \xi_i)$. This equation states that ξ_μ is characteristic, with ξ_0 a root of the *characteristic polynomial* $\det \mathcal{P}(\xi)$. This is a polynomial of degree $2N$ in ξ_0 hence there are $2N$ (possibly degenerate) eigenvalues ξ_0 and $2N$ corresponding characteristic covectors ξ_μ. Strong hyperbolicity requires that these eigenvalues are all real and (in the case of degeneracy) that the algebraic multiplicity of each eigenvalue is equal to its geometric multiplicity (the dimension of the space of solutions t_I to (3.18)).

The contracted Bianchi identity implies, for any ξ_μ,

$$\mathcal{P}_\star(\xi)^{\mu\nu\rho\sigma} \xi_\nu = 0 \tag{3.19}$$

Hence contracting (3.18) with ξ_ν gives

$$0 = \mathcal{P}_{\rm GF}(\xi)^{\mu\nu\rho\sigma} \xi_\nu t_{\rho\sigma} = -\frac{1}{2}(\hat{g}^{\nu\gamma}\xi_\nu\xi_\gamma)(g^{\mu\beta}\tilde{P}_\beta{}^{\delta\rho\sigma}\xi_\delta t_{\rho\sigma}) \tag{3.20}$$

So the analysis splits into two cases: either (i) $\tilde{P}_\beta{}^{\delta\rho\sigma}\xi_\delta t_{\rho\sigma} = 0$ or (ii) $\hat{g}^{\nu\gamma}\xi_\nu\xi_\gamma = 0$.

Case (i) is defined by

$$\tilde{P}_\beta{}^{\delta\rho\sigma}\xi_\delta t_{\rho\sigma} = 0 \tag{3.21}$$

Physically, this case corresponds to a high-frequency wave with wavevector ξ_μ and polarization t_I that satisfies the gauge condition (3.4). The condition (3.21) implies

$\mathcal{P}_{\rm GF}(\xi)t = 0$ and so (3.18) reduces to

$$\mathcal{P}_\star(\xi)^{\mu\nu\rho\sigma}t_{\rho\sigma} = 0 \tag{3.22}$$

We can divide the analysis into two subcases.

Subcase (ia) is defined by $g^{\gamma\delta}\xi_\gamma\xi_\delta \neq 0$. Equation (3.22) contains a term $-\frac{1}{2}g^{\gamma\delta}\xi_\gamma\xi_\delta t^{\mu\nu}$ and all other terms have the form $Y^{(\mu}\xi^{\nu)}$ for some Y^μ (depending on t), or are proportional to $g^{\mu\nu}$. It follows that $t_{\mu\nu}$ must have the form

$$t_{\mu\nu} = X_{(\mu}\xi_{\nu)} + cg_{\mu\nu} \tag{3.23}$$

for some X_μ and c. Equation (3.22) now reduces to $c\left(g^{\gamma\delta}\xi_\gamma\xi_\delta g^{\mu\nu} - \xi^\mu\xi^\nu\right) = 0$ so $c = 0$. Assuming $t_{\mu\nu} \neq 0$ (i.e. $X_\mu \neq 0$), equation (3.21) now reduces to

$$\tilde{g}^{\mu\nu}\xi_\mu\xi_\nu = 0 \tag{3.24}$$

Our requirement that the null cones of $g^{\mu\nu}$ and $\tilde{g}^{\mu\nu}$ do not intersect implies that this is consistent with our starting assumption $g^{\gamma\delta}\xi_\gamma\xi_\delta \neq 0$.

Since our surfaces of constant x^0 are spacelike w.r.t. $\tilde{g}^{\mu\nu}$, (3.24) admits two real solutions $\tilde{\xi}_0^\pm$ which depend smoothly on ξ_i. We write the corresponding characteristic covectors as $\tilde{\xi}_\mu^\pm = (\tilde{\xi}_0^\pm, \xi_i)$, and these are null w.r.t. $\tilde{g}^{\mu\nu}$. The choice of $\pm$ corresponds to this null covector lying on either the future or past null cone of $\tilde{g}^{\mu\nu}$. Since dx^0 is timelike w.r.t. $\tilde{g}^{\mu\nu}$ we can distinguish these two possibilities by the sign of the non-zero quantity $(dx^0)_\mu\tilde{g}^{\mu\nu}\tilde{\xi}_\nu^\pm = \tilde{g}^{0\nu}\tilde{\xi}_\nu^\pm$. Our convention is that $\mp\tilde{g}^{0\nu}\tilde{\xi}_\nu^\pm > 0$.

The corresponding eigenvectors are $t_{\mu\nu} = X_{(\mu}\tilde{\xi}_{\nu)}^\pm$ where X_μ is an arbitrary covector. These are "pure gauge" eigenvectors, arising from a residual gauge freedom of (3.7). Note that in this case we have d linearly independent eigenvectors for each eigenvalue $\tilde{\xi}_0^\pm$.

Subcase (ib) is defined by

$$g^{\mu\nu}\xi_\mu\xi_\nu = 0 \tag{3.25}$$

Since surfaces of constant x^0 are spacelike w.r.t. $g^{\mu\nu}$ this equation admits two real solutions $\xi_0^\pm$ depending smoothly on ξ_i. The characteristic covector is $\xi_\mu^\pm = (\xi_0^\pm, \xi_i)$, which is null w.r.t. $g^{\mu\nu}$. We fix the signs as in case (ia) by demanding that $\mp\xi^{\pm 0} =$

$\mp g^{0\nu}\xi_\nu^\pm > 0$. The equation $\mathcal{P}_\star(\xi)t = 0$ reduces to

$$P_\beta{}^{\delta\rho\sigma}\xi_\delta^\pm t_{\rho\sigma} = 0 \tag{3.26}$$

This says that the "polarization" $t_{\mu\nu}$ is transverse w.r.t. $g^{\mu\nu}$. (Note that we should really include a $\pm$ superscript on $t_{\mu\nu}$ but we suppress this to ease the notation.) However, the defining condition of case (i) gives

$$\tilde{P}_\beta{}^{\delta\rho\sigma}\xi_\delta^\pm t_{\rho\sigma} = 0 \tag{3.27}$$

so the polarization is also transverse w.r.t. $\tilde{g}^{\mu\nu}$. In order to solve these conditions we can introduce a basis $\{e_0, e_1, e_{\hat{i}}, \hat{i} = 2, \ldots, d-1\}$ for the tangent space such that $(e_0)^\mu = \xi^{\pm\mu}$ and $e_1^\mu \propto \xi^{\mp\mu}$, so e_0 and e_1 are both null w.r.t. $g_{\mu\nu}$. The normalization of e_1, and the other (spacelike) basis vectors are chosen so that

$$g(e_0, e_1) = 1 \qquad\qquad g(e_{\hat{i}}, e_{\hat{j}}) = \delta_{\hat{i}\hat{j}} \tag{3.28}$$

and all other inner products of basis vectors w.r.t. g vanish. Since $\xi_\mu^\pm$ depends smoothly on ξ_i, our basis can be chosen to depend smoothly on ξ_i. In such a basis, equation (3.26) reduces to $t_{00} = t_{0\hat{i}} = t_{\hat{i}\hat{i}} = 0$. Since the null cones of $g^{\mu\nu}$ and $\tilde{g}^{\mu\nu}$ do not intersect, it follows that $0 \neq \tilde{g}^{\mu\nu}\xi_\mu^\pm\xi_\nu^\pm = \tilde{g}^{11}$. Using this, equation (3.27) reduces to $t_{01} = 0$ and

$$t_{11} = (\tilde{g}^{11})^{-1}\tilde{g}^{\hat{i}\hat{j}}t_{\hat{i}\hat{j}} \qquad t_{1\hat{i}} = (\tilde{g}^{11})^{-1}\tilde{g}^{1\hat{j}}t_{\hat{i}\hat{j}} \tag{3.29}$$

In summary, we have shown that

$$t_{0\mu} = t_{\hat{i}\hat{i}} = 0 \tag{3.30}$$

and all components of $t_{\mu\nu}$ are determined (via (3.29)) by the traceless quantity $t_{\hat{i}\hat{j}}$, which has $(1/2)d(d-3)$ independent components. Hence, for each eigenvalue $\xi_0^\pm$, $t_{\mu\nu}$ has $(1/2)d(d-3)$ independent components so the corresponding eigenspace has dimension $d(d-3)/2$. This is the number of degrees of freedom of a graviton, so these eigenvectors correspond to physical polarizations. If we choose a set of linearly independent eigenvectors for which $t_{\hat{i}\hat{j}}$ is independent of ξ_i then these eigenvectors will depend smoothly on ξ_i.

Case (ii) is defined by

$$\hat{g}^{\nu\gamma}\xi_\nu\xi_\gamma = 0 \tag{3.31}$$

Since our surfaces of constant x^0 are spacelike w.r.t. $\hat{g}^{\mu\nu}$, it follows that this equation admits two real solutions $\hat{\xi}_0^{\pm}$. We write the characteristic covector as $\hat{\xi}_\mu = (\hat{\xi}_0^{\pm}, \xi_i)$ and fix the signs as in the previous cases by requiring that $\mp\hat{g}^{0\nu}\hat{\xi}_\nu^{\pm} > 0$.

Recall (from (3.19) and (3.20)) that (3.31) guarantees that the contraction of (3.18) with $\hat{\xi}_\nu^{\pm}$ is satisfied, i.e., d components of (3.18) are trivial. So (3.18) is $d(d+1)/2 - d$ linear equations involving the $d(d+1)/2$ components of $t_{\mu\nu}$. It follows that there must exist at least d linearly independent solutions $t_{\mu\nu}$ for each eigenvalue $\hat{\xi}_0^{\pm}$. We can see that there exist exactly d such solutions simply by counting the number of eigenvectors we have already determined. We have $2d$ eigenvectors in case (ia) (d for each eigenvalue $\tilde{\xi}_0^{\pm}$) and $d(d-3)$ eigenvectors in case (ib) ($d(d-3)/2$ for each eigenvalue $\xi_0^{\pm}$). So we have already found $d(d-1)$ eigenvectors in case (i). The total number of eigenvectors of $M(\xi_i)$ cannot exceed $2N = d(d+1)$ so we can have at most $2d$ eigenvectors in case (ii). Since we have at least d eigenvectors for each eigenvalue $\hat{\xi}_0^{\pm}$ it follows that we must have *exactly* d eigenvectors for each of these eigenvalues. Since these eigenvectors are associated with characteristics that are null w.r.t. $\hat{g}^{\mu\nu}$, i.e., the same as the characteristics of (3.8), we interpret these eigenvectors as describing "gauge-condition violating" polarizations.

We can construct these eigenvectors as follows. Since $\hat{\xi}_\mu^{\pm}$ is null w.r.t. $\hat{g}^{\mu\nu}$, it is spacelike w.r.t. $g^{\mu\nu}$. We now introduce a basis $\{e_0^\mu, e_1^\mu, \dots, e_{d-1}^\mu\}$ of vectors that are orthonormal w.r.t. $g_{\mu\nu}$. We choose this basis so that e_1^μ is in the direction of the spacelike vector $\hat{\xi}^{\pm\mu}$. This orthonormal basis can be chosen so that the basis vectors depend smoothly on ξ_i.[2]

We define indices $A, B, \dots$ to take values $0, 2, 3, \dots, d-1$. As just discussed, the contraction of (3.18) with $\hat{\xi}_\mu^{\pm}$ is trivial so, in our basis, only the AB components of this equation are non-trivial. Furthermore, (3.19) implies that the only non-vanishing components of $\mathcal{P}_\star(\hat{\xi}^{\pm})^{\mu\nu\rho\sigma}$ are $\mathcal{P}_\star(\hat{\xi}^{\pm})^{ABCD}$.

In this basis, a general symmetric tensor can be written as

$$t_{\mu\nu} = \hat{\xi}_{(\mu}^{\pm} X_{\nu)} + t_{AB} e_\mu^A e_\nu^B \tag{3.32}$$

where the 1μ components of t are proportional to the vector X_μ of the first term. Note that this first term is in the kernel of $\mathcal{P}_\star(\hat{\xi}^{\pm})$.

[2] To see this, start from some fixed orthonormal basis. Perform a rotation of the spatial basis vectors so that the spatial part of $\hat{\xi}^{\pm\mu}$ is in the direction e_1^μ. Now perform a boost in the 1-direction to eliminate the time component of $\hat{\xi}^{\pm\mu}$. The rotation and boost will depend smoothly on ξ_i hence the new basis depends smoothly on ξ_i.

To construct the eigenvectors, let v^μ be an arbitrary vector. Consider the equation

$$\mathcal{P}_\star(\hat{\xi}^\pm)^{ABCD} t_{CD} = \hat{P}_\alpha{}^{\beta AB} \hat{\xi}^\pm_\beta v^\alpha \tag{3.33}$$

We claim that this can be uniquely solved for t_{AB}. We will show that $\mathcal{P}_\star(\hat{\xi}^\pm)^{ABCD}$ has trivial kernel and is therefore invertible. So assume that s_{AB} belongs to this kernel, i.e.,

$$\mathcal{P}_\star(\hat{\xi}^\pm)^{ABCD} s_{CD} = 0 \tag{3.34}$$

This implies that, for any $s_{1\mu}$,

$$\mathcal{P}_\star(\hat{\xi}^\pm)^{\mu\nu\rho\sigma} s_{\rho\sigma} = 0 \tag{3.35}$$

This is the same as equation (3.22) that we encountered in case (i) and can be solved as in subcase (ia). Using the fact that $\hat{\xi}^\pm_\mu$ is non-null w.r.t. $g^{\mu\nu}$, it follows from the tensorial structure of the equation that any such $s_{\rho\sigma}$ must have the form $s_{\rho\sigma} = c\, g_{\rho\sigma} + \hat{\xi}^\pm_{(\rho} Y_{\sigma)}$ for some c and Y_σ. Substituting this into (3.35) gives $c = 0$. Hence $s_{\mu\nu}$ must be "pure gauge", i.e., the only non-trivial components are $s_{1\mu}$. In particular $s_{AB} = 0$ so the kernel of $\mathcal{P}_\star(\hat{\xi}^\pm)^{ABCD}$ is trivial as claimed. Hence (3.33) can be solved uniquely for t_{AB}. Furthermore, since the matrix on the LHS depends smoothly on ξ_i, it follows that the solution t_{AB} will depend smoothly on ξ_i and v^μ. We also have

$$\mathcal{P}_\star(\hat{\xi}^\pm)^{\mu\nu\rho\sigma} t_{\rho\sigma} = \hat{P}_\alpha{}^{\beta\mu\nu} \hat{\xi}^\pm_\beta v^\alpha \tag{3.36}$$

because both sides have vanishing contraction with $\hat{\xi}^\pm_\mu$ and hence with the basis vector e_1.

Next we fix X_μ by requiring that

$$\tilde{P}^{\mu\nu\rho\sigma} \hat{\xi}^\pm_\nu t_{\rho\sigma} = v^\mu \tag{3.37}$$

This equation can be solved uniquely for X_μ in terms of v^μ and t_{AB}. To see this, note that the action of $\tilde{P}^{\mu\nu\rho\sigma}\hat{\xi}^\pm_\nu$ on $\hat{\xi}^\pm_{(\rho} X_{\sigma)}$ is

$$\tilde{P}^{\mu\nu\rho\sigma} \hat{\xi}^\pm_\nu \hat{\xi}^\pm_{(\rho} X_{\sigma)} = \frac{1}{2}\left(\tilde{g}^{\gamma\delta} \hat{\xi}^\pm_\gamma \hat{\xi}^\pm_\delta\right) X^\mu. \tag{3.38}$$

On the RHS, we know that $\hat{\xi}^{\pm}_{\mu}$ is non-null w.r.t. $\tilde{g}^{\mu\nu}$ because the null cones of $\tilde{g}^{\mu\nu}$ and $\hat{g}^{\mu\nu}$ do not intersect. Hence (3.37) determines X^{μ} in terms of v^{μ} and t_{AB}:

$$X^{\mu}(v, t_{AB}) = \frac{2}{\tilde{g}^{\gamma\delta}\hat{\xi}^{\pm}_{\gamma}\hat{\xi}^{\pm}_{\delta}} \left(v^{\mu} - \tilde{P}^{\mu\nu AB}\hat{\xi}^{\pm}_{\nu}\ t_{AB} \right) \tag{3.39}$$

Let $t_{AB}(v)$ denote the solution of (3.33) and let

$$t_{\mu\nu}(v) = \hat{\xi}^{\pm}_{(\mu} X_{\nu)}(v, t_{AB}(v)) + t_{AB}(v) e^{A}_{\mu} e^{B}_{\nu}. \tag{3.40}$$

This satisfies (3.18) because

$$\begin{aligned} \mathcal{P}(\hat{\xi}^{\pm})^{\mu\nu\rho\sigma} t_{\rho\sigma}(v) &= \left(\mathcal{P}_{\star}(\hat{\xi}^{\pm})^{\mu\nu\rho\sigma} - \hat{P}_{\alpha}{}^{\beta\mu\nu}\hat{\xi}^{\pm}_{\beta}\tilde{P}^{\alpha\gamma\rho\sigma}\hat{\xi}^{\pm}_{\gamma} \right) t_{\rho\sigma}(v) \\ &= \hat{P}_{\alpha}{}^{\beta\mu\nu}\hat{\xi}^{\pm}_{\beta}\ v^{\alpha} - \hat{P}_{\alpha}{}^{\beta\mu\nu}\hat{\xi}^{\pm}_{\beta}\tilde{P}^{\alpha\gamma\rho\sigma}\hat{\xi}^{\pm}_{\gamma} t_{\rho\sigma}(v) = 0 \end{aligned} \tag{3.41}$$

where we used (3.36) in the second equality and (3.37) in the third.

For every v^{μ} we have constructed a solution $t_{\mu\nu}$ of (3.18) that depends smoothly on v^{μ} and ξ_i. If we choose a set of d linearly independent vectors v^{μ} then the corresponding t_{AB} are also linearly independent (using the triviality of the kernel mentioned above), and so the resulting $t_{\mu\nu}$ are linearly independent. Thus, for each eigenvalue $\hat{\xi}^{\pm}_{0}$, we have constructed a set of d linearly independent eigenvectors depending smoothly on ξ_i.

In summary, the above calculation shows that $M(\xi_i)$ has 6 distinct eigenvalues, namely $\xi^{\pm}_{0}$, $\tilde{\xi}^{\pm}_{0}$ and $\hat{\xi}^{\pm}_{0}$. These are all real. We have also shown that $M(\xi_i)$ has a full set of $2N$ linearly independent eigenvectors depending smoothly on ξ_i. Hence we have established that (3.7) is strongly hyperbolic.

3.3 Lovelock theories

3.3.1 Principal symbol

We define the modified harmonic gauge equation of motion of a Lovelock theory in exactly the same way as in GR. We start from the equation of motion in the form (1.8) and add a gauge fixing term as in (3.5) to obtain the modified harmonic gauge equation of motion in the form (3.7), i.e.,

$$E^{\mu\nu}_{\text{mhg}} \equiv E^{\mu\nu} + \hat{P}_{\alpha}{}^{\beta\mu\nu}\partial_{\beta}H^{\alpha} = 0 \tag{3.42}$$

Initial data for (3.42) consists, as in GR, of a triple $(\Sigma, h_{\mu\nu}, K_{\mu\nu})$ which must satisfy the constraint equations arising from (1.8).

The auxiliary metrics $\tilde{g}^{\mu\nu}$ and $\hat{g}^{\mu\nu}$ are chosen in the same way as in GR and we continue to raise/lower indices using $g^{\mu\nu}$ and $g_{\mu\nu}$. The argument for the propagation of the gauge condition is identical to GR (section 3.2.2) since it uses only the Bianchi identity for $E^{\mu\nu}$, which continues to hold in Lovelock theories.

The Lovelock equation of motion is not quasilinear, i.e., it is not linear in 2nd derivatives. We define the principal symbol as explained in section 1.2. The result can be written as in (3.9) where the gauge-fixing term is (3.11) and the matrix $\mathcal{P}_\star(\xi)$ now takes the form [59, 60, 92]

$$\begin{aligned} \mathcal{P}_\star(\xi)^{\mu\nu\rho\sigma}t_{\rho\sigma} &= -\frac{1}{2}g^{\gamma\delta}\xi_\gamma\xi_\delta P^{\mu\nu\rho\sigma}t_{\rho\sigma} + P_\alpha{}^{\gamma\mu\nu}\xi_\gamma g^{\alpha\beta}P_\beta{}^{\delta\rho\sigma}\xi_\delta t_{\rho\sigma} \\ &\quad -2\sum_{p\geq 2} p\ k_p\ \delta^{\mu\rho\gamma\alpha_3\alpha_4\ldots\alpha_{2p-1}\alpha_{2p}}_{\nu\sigma\delta\beta_3\beta_4\ldots\beta_{2p-1}\beta_{2p}} t_\rho{}^\sigma \xi_\gamma \xi^\delta R_{\alpha_3\alpha_4}{}^{\beta_3\beta_4} \ldots\ R_{\alpha_{2p-1}\alpha_{2p}}{}^{\beta_{2p-1}\beta_{2p}}. \end{aligned} \tag{3.43}$$

In this equation, the terms in the first line arise from the Einstein tensor and the second line is the Lovelock contribution.

We can now explain what we mean by the theory being "weakly coupled". The Lovelock coupling constants k_p are dimensionful. "Weakly coupled" means that the spacetime curvature is small compared to the scales defined by these constants. More precisely, it means that the terms on the second line of (3.43) are small compared to the terms on the first line (which don't involve the curvature). If our initial data is such that this assumption is satisfied then, by continuity, a solution of (3.42) arising from this data will continue to be weakly coupled in a neighbourhood of Σ. However, the theory may become strongly coupled when one considers evolution over larger time intervals. For example, the theory would become strongly coupled if a curvature singularity forms. At strong coupling, well-posedness can fail [59].

Although not quasilinear, Lovelock theories have the special property that, in any coordinate chart, the equation of motion *is* linear in the second derivative w.r.t. any given coordinate[3] [92, 93], and this property is not affected by the gauge fixing term.

[3] To see this, note that the only Riemann tensor components that contain second derivatives w.r.t. x^α are $R_{\alpha\mu\alpha\nu}$ and components related by antisymmetry (no summation on α). In (1.8), the antisymmetrization over $\rho_1, \ldots, \rho_{2p}$ implies that at most one of these indices can take the value α. Hence there are no products of second derivatives w.r.t. x^α.

So in a chart x^μ the modified harmonic gauge equation of motion takes the form

$$A^{IJ}(x, g, \partial_\mu g, \partial_0\partial_i g, \partial_i\partial_j g)\partial_0^2 g_J = F^I(x, g, \partial_\mu g, \partial_0\partial_i g, \partial_i\partial_j g) \tag{3.44}$$

where we are using the notation of section 3.2.3 in which indices $I, J, \ldots$ label a symmetric tensor so g_I is the physical metric. A^{IJ} is defined in terms of $P(\xi)$ as in (3.15). The point is that the above equation is linear in $\partial_0^2 g_I$. A surface of constant x^0 is non-characteristic iff the matrix A^{IJ} is invertible on that surface. Recall that in GR this is guaranteed if the surface is spacelike w.r.t. $g^{\mu\nu}$, so $\det A^{IJ} \neq 0$ on such a surface in GR. By continuity, we must also have $\det A^{IJ} \neq 0$ on a spacelike surface in Lovelock theory provided the theory is sufficiently weakly coupled.

For non-quasilinear equations with the special property just described, the initial value problem is well-posed for initial data prescribed on a (non-characteristic) surface of constant x^0 provided that the equation of motion is strongly hyperbolic. (For more details, see section 1.2.) Thus to establish well-posedness we just need to demonstrate that our modified harmonic gauge Lovelock equation of motion (3.42) is strongly hyperbolic.

3.3.2 Proof of strong hyperbolicity

Our proof follows closely the analysis (and notation) of section 3.2.3. We define the matrices A^{IJ}, B^{IJ} and C^{IJ} in terms of the principal symbol as in (3.15) and then define $M(\xi_i)$ with (3.16). We want to show that this matrix satisfies the conditions for strong hyperbolicity reviewed in section 3.2.3. At weak coupling, this matrix will be close to the corresponding matrix for GR. Several steps of our argument will exploit continuity to deduce that certain features of $M(\xi_i)$ are preserved when we deform from GR to a weakly coupled Lovelock theory.

For modified harmonic gauge GR, we showed that $M(\xi_i)$ has 6 distinct eigenvalues. At sufficiently weak coupling, the Lovelock terms give a small deformation of the matrix $M(\xi_i)$. Since the eigenvalues of $M(\xi_i)$ depend continuously on $M(\xi_i)$, the resulting eigenvalues will fall into 6 groups, which (following [94]) we call the ξ_0^+-group, the ξ_0^--group etc. Note that this division is possible only at weak coupling.

At this stage we do not know that the eigenvalues of $M(\xi_i)$ are real so we view $M(\xi_i)$ as acting on the $2N$-dimensional vector space V of *complex* vectors of the form $v = (t_{\mu\nu}, t'_{\mu\nu})^T$ where $t_{\mu\nu}$ and $t'_{\mu\nu}$ are symmetric. For each eigenvalue λ we can define a "generalized eigenspace". This is the space of vectors v satisfying $(M(\xi_i) - \lambda)^k v = 0$

for some $k \in \{1, 2, \ldots\}$. It corresponds to the sum of the Jordan blocks of $M(\xi_i)$ that have eigenvalue λ. We then define the "total generalized eigenspace" associated to the ξ_0^+-group as the direct sum of the generalized eigenspaces of each eigenvalue in the ξ_0^+-group, and similarly for the other groups [94]. This gives the decomposition

$$V = V^+ \oplus \tilde{V}^+ \oplus \hat{V}^+ \oplus V^- \oplus \tilde{V}^- \oplus \hat{V}^- \tag{3.45}$$

where V^+ is the total generalized eigenspace associated to ξ_0^+-group etc. Note that these spaces depend on ξ_i. In GR these spaces are simply the eigenspaces associated to each eigenvalue.

We define the matrix [94]

$$\Pi^+ = \frac{1}{2\pi i} \int_{\Gamma^+} (M(\xi_i) - z)^{-1} dz \tag{3.46}$$

where Γ^+ is a circle (traversed anticlockwise) in the complex z-plane that encloses the point $z = \xi_0^+$ and is sufficiently small that only the eigenvalues of the ξ_0^+ group lie inside this circle, with all other eigenvalues lying outside this circle. The residue theorem implies that $\Pi^+ : V \to V$ is a projection onto V^+. We can define similar projections $\tilde{\Pi}^+$ etc onto the other eigenspaces. Note that these projection operators are *smooth* functions of ξ_i, the background curvature, the Lovelock couplings etc. Note that the dimension of V^+ is the trace of Π^+. By continuity, this is the same for weakly coupled Lovelock theory as for GR and similarly for the dimensions of the other spaces in (3.45). Hence we know that $V^\pm$ have dimension $(1/2)d(d-3)$ and the other spaces have dimension d.

Equation (3.19) is a consequence of the Bianchi identity for $E^{\mu\nu}$ and therefore holds in a Lovelock theory. This implies that the argument leading to (3.20) is valid for Lovelock theory. Thus the analysis splits into case (i) and case (ii) just as in GR.

We start by observing that the (real) "pure gauge" eigenvectors of subcase (ia) are also eigenvectors for Lovelock theory, with the same (real) eigenvalues $\tilde{\xi}_0^\pm$. To see this, note that these eigenvectors have $t_{\mu\nu} = X_{(\mu}\tilde{\xi}^\pm_{\nu)}$, which, because of the antisymmetrization, gives a vanishing contribution to the second line of (3.43) (with $\xi_\mu = \tilde{\xi}^\pm_\mu$). Therefore the principal symbol acts on such $t_{\mu\nu}$ in exactly the same way as in GR so these eigenvectors are the same as in GR. This shows that the spaces $\tilde{V}^\pm$ are genuine eigenspaces spanned by these eigenvectors. We will discuss the Lovelock generalization of subcase (ib) (the physical eigenvectors) below.

In case (ii) the analysis proceeds similarly to GR. This case is defined by (3.31), so the (real) eigenvalues are $\hat{\xi}_0^{\pm}$, exactly as in GR. To construct the eigenvectors we proceed as in GR. The only step where the argument needs modifying is the demonstration that the kernel of $\mathcal{P}_\star^{ABCD}$ is trivial. We showed that this kernel is trivial for GR so $\mathcal{P}_\star^{ABCD}$ has non-vanishing determinant in GR. By continuity the determinant must remain non-zero in weakly coupled Lovelock theory. Hence the kernel is trivial for weakly coupled Lovelock theory. The rest of the argument is identical to the argument for GR. Hence one obtains d real smooth eigenvectors for each eigenvalue $\hat{\xi}_0^{\pm}$. The spaces $\hat{V}^{\pm}$ are therefore genuine eigenspaces.

It remains to discuss the "physical" eigenvalues of the $\xi_0^{\pm}$-groups, which correspond to subcase (ib) of the GR analysis. Generically the eigenvalues of the $\xi_0^{\pm}$ group will be non-degenerate, unlike the cases just discussed. Roughly speaking, this corresponds to the fact that, in a Lovelock theory, gravitational waves with different polarizations travel (in a non-trivial background) with different speeds [59]. We will not attempt to construct the eigenvectors directly in this case. Instead we will construct an inner product on $V^{\pm}$ which we will use to build a symmetrizer for $M(\xi_i)$.

We start by defining the matrices

$$H_\star^{\pm} = \pm \begin{pmatrix} B_\star & A_\star \\ A_\star & 0 \end{pmatrix} \tag{3.47}$$

where $A_\star$ and $B_\star$ are defined as in (3.15) but using $\mathcal{P}_\star$ instead of $\mathcal{P}$. We use these matrices to define a Hermitian form $(,)_\pm$ on $V^{\pm}$ as follows:

$$(v^{(1)}, v^{(2)})_\pm = v^{(1)\dagger} H_\star^{\pm} v^{(2)} \tag{3.48}$$

where $v^{(1)}$ and $v^{(2)}$ are in $V^{\pm}$. This is Hermitian because $B_\star$ and $A_\star$ are real symmetric matrices (because $\mathcal{P}_\star$ is real symmetric) so $H_\star^{\pm}$ is also real symmetric. We will now show that this Hermitian form is positive definite and therefore defines an inner product. To do this we will show that it is positive definite for GR. By continuity (of the eigenvalues of the Hermitian form) it then follows that it is also positive definite for a weakly coupled Lovelock theory.

In GR, the spaces $V^{\pm}$ are genuine eigenspaces with eigenvalue $\xi_0^{\pm}$, which implies that we have $v^{(1)} = (t^{(1)}, \xi_0^{\pm} t^{(1)})^T$ and similarly for $v^{(2)}$. This implies that, in GR[4]

$$\begin{aligned}
(v^{(1)}, v^{(2)})_{\pm} &= \pm t^{(1)*}_{\mu\nu} (2\xi_0^{\pm} A_\star + B_\star)^{\mu\nu\rho\sigma} t^{(2)}_{\rho\sigma} \\
&= \pm t^{(1)*}_{\mu\nu} \left[-g^{0\gamma} \xi^{\pm}_{\gamma} P^{\mu\nu\rho\sigma} + P_{\alpha}{}^{0\mu\nu} P^{\alpha\gamma\rho\sigma} \xi^{\pm}_{\gamma} + P_{\alpha}{}^{\gamma\mu\nu} \xi^{\pm}_{\gamma} P^{\alpha 0\rho\sigma} \right] t^{(2)}_{\rho\sigma} \\
&= \mp \xi^{\pm 0} t^{(1)*}_{\mu\nu} P^{\mu\nu\rho\sigma} t^{(2)}_{\rho\sigma} \qquad (3.49)
\end{aligned}$$

where in the final step we used the fact that $v^{(1)}$ and $v^{(2)}$ belong to $V^{\pm}$ so $t^{(1)}$ and $t^{(2)}$ satisfy the condition (3.26). Finally, evaluating this in the null basis we used to discuss case (ib) above, and using (3.29) and (3.30) we obtain

$$(v^{(1)}, v^{(2)})_{\pm} = \mp \xi^{\pm 0} t^{(1)*}_{\hat{i}\hat{j}} t^{(2)}_{\hat{i}\hat{j}} \qquad (3.50)$$

Since $t_{1\mu}$ is determined in terms of $t_{\hat{i}\hat{j}}$ by (3.29), and $\mp\xi^{\pm 0} > 0$, this is indeed a positive definite Hermitian form on $V^{\pm}$. Having established this for GR, the result then follows for a weakly coupled Lovelock theory by continuity.

Our next task is to show that the eigenvalues belonging to the $\xi_0^{\pm}$ groups are real. Consider two eigenvalues $\xi_0^{(1)}$ and $\xi_0^{(2)}$ belonging to the ξ_0^{+}-group, with corresponding eigenvectors $v^{(1)} = (t^{(1)}, \xi_0^{(1)} t^{(1)})^T$ and $v^{(2)} = (t^{(2)}, \xi_0^{(2)} t^{(2)})^T$. The eigenvalues and eigenvectors may be complex. Since these eigenvectors belong to case (i) they satisfy the condition

$$\tilde{P}_{\beta}{}^{\delta\rho\sigma} \xi^{(1)}_{\delta} t^{(1)}_{\rho\sigma} = 0 \qquad (3.51)$$

where $\xi^{(1)}_{\delta} = (\xi^{(1)}_0, \xi_i)$, and similarly for $t^{(2)}$. We now have

$$\begin{aligned}
\left(\xi_0^{(1)} - \xi_0^{(2)}\right) v^{(1)T} H^{+}_{\star} v^{(2)} &= t^{(1)}_{\mu\nu} \left[\left(\xi_0^{(1)2} - \xi_0^{(2)2}\right) A_\star + \left(\xi_0^{(1)} - \xi_0^{(2)}\right) B_\star \right]^{\mu\nu\rho\sigma} t^{(2)}_{\rho\sigma} \\
&= t^{(1)}_{\mu\nu} \left[\mathcal{P}_\star(\xi^{(1)}) - \mathcal{P}_\star(\xi^{(2)}) \right]^{\mu\nu\rho\sigma} t^{(2)}_{\rho\sigma} \\
&= t^{(2)}_{\mu\nu} \mathcal{P}_\star(\xi^{(1)})^{\mu\nu\rho\sigma} t^{(1)}_{\rho\sigma} - t^{(1)}_{\mu\nu} \mathcal{P}_\star(\xi^{(2)})^{\mu\nu\rho\sigma} t^{(2)}_{\rho\sigma} \\
&= t^{(2)}_{\mu\nu} \mathcal{P}(\xi^{(1)})^{\mu\nu\rho\sigma} t^{(1)}_{\rho\sigma} - t^{(1)}_{\mu\nu} \mathcal{P}(\xi^{(2)})^{\mu\nu\rho\sigma} t^{(2)}_{\rho\sigma} = 0 \qquad (3.52)
\end{aligned}$$

The second equality uses the definition of $A_\star$ and $B_\star$, the third equality uses the symmetry of $\mathcal{P}_\star$. The fourth equality follows from (3.51) which implies that $t^{(1)}$ is in the kernel of $\mathcal{P}_{\mathrm{GF}}(\xi^{(1)})$ and similarly for $t^{(2)}$. The final equality follows from (3.18).

Assume that the ξ_0^{+}-group contains an eigenvalue ξ_0 with $\mathrm{Im}(\xi_0) \neq 0$ and corresponding eigenvector v (belonging to V^{+}). Since $M(\xi_i)$ is real, it follows that ξ_0^* is also an

[4] Note that we use $*$ to denote a complex conjugate, which is different from the label $\star$ on $A_\star$ etc.

eigenvalue, with eigenvector v^*. We now set $\xi_0^{(1)} = \xi_0^*$, $v^{(1)} = v^*$, $\xi_0^{(2)} = \xi_0$ and $v^{(2)} = v$ to deduce from the above that

$$v^\dagger H_\star^+ v = 0 \tag{3.53}$$

i.e. $(v,v)_+ = 0$. But we have already seen that $(,)_+$ is positive definite in V^+ and so this equation implies that $v = 0$, a contradiction. Hence the eigenvalues in the ξ_0^+-group are all real and similarly for the ξ_0^- group.

Finally we need to show that $M(\xi_i)$ is diagonalizable. Note that we have already constructed d eigenvectors in each of the spaces $\tilde{V}^\pm$ and $\hat{V}^\pm$. So we just need to show that $M(\xi_i)$ is diagonalizable in $V^\pm$. To do this we need more information about the elements of $V^\pm$. Note in particular that a general element of $V^\pm$ is *not* an eigenvector, unlike the case of GR.

Consider the *left* eigenvectors of $M(\xi_i)$. The left eigenvalues of a matrix are the same as its right eigenvalues. A simple calculation reveals that a left eigenvector with eigenvalue ξ_0 has the form

$$w = (s_I, \xi_0 s_I) \begin{pmatrix} B & A \\ A & 0 \end{pmatrix} \tag{3.54}$$

where

$$s_{\mu\nu} P(\xi)^{\mu\nu\rho\sigma} = 0 \tag{3.55}$$

A family of left eigenvectors with eigenvalue $\hat{\xi}_0^\pm$ is obtained by choosing

$$s_{\mu\nu} = X_{(\mu}\hat{\xi}^\pm_{\nu)} \tag{3.56}$$

Now, from the Jordan canonical form of $M(\xi_i)$ it follows that a vector $v = (t_I, t'_I)$ in any of the spaces V^+, V^-, $\tilde{V}^+$ or $\tilde{V}^-$ must be orthogonal to these left eigenvectors in the sense that

$$0 = wv = s_{\mu\nu} \left(B + \hat{\xi}_0^\pm A\right)^{\mu\nu\rho\sigma} t_{\rho\sigma} + s_{\mu\nu} A^{\mu\nu\rho\sigma} t'_{\rho\sigma} \tag{3.57}$$

Since X_μ is arbitrary, this implies

$$0 = \hat{\xi}^\pm_\nu \left(B + \hat{\xi}_0^\pm A\right)^{\mu\nu\rho\sigma} t_{\rho\sigma} + \hat{\xi}^\pm_\nu A^{\mu\nu\rho\sigma} t'_{\rho\sigma} \tag{3.58}$$

This expression has to hold for both sign choices $\pm$. Note that it is quadratic in $\hat{\xi}_0^\pm$. We can eliminate $(\hat{\xi}_0^\pm)^2$ using the defining equation (3.31), to obtain

$$\hat{\xi}_0^\pm R^\mu + S^\mu = 0 \tag{3.59}$$

where

$$R^\mu = -2\left(\hat{g}^{00}\right)^{-1}\hat{g}^{0i}\xi_i A^{\mu 0\rho\sigma}t_{\rho\sigma} + B^{\mu 0\rho\sigma}t_{\rho\sigma} + \xi_i A^{\mu i\rho\sigma}t_{\rho\sigma} + A^{\mu 0\rho\sigma}t'_{\rho\sigma} \tag{3.60}$$

and

$$S^\mu = -\left(\hat{g}^{00}\right)^{-1}\hat{g}^{ij}\xi_i\xi_j A^{\mu 0\rho\sigma}t_{\rho\sigma} + \xi_i B^{\mu i\rho\sigma}t_{\rho\sigma} + \xi_i A^{\mu i\rho\sigma}t'_{\rho\sigma} \tag{3.61}$$

(Recall that $\hat{g}^{00} \neq 0$ because our surfaces of constant x^0 are spacelike w.r.t. $g^{\mu\nu}$ and hence spacelike w.r.t. $\hat{g}^{\mu\nu}$.) Since $\hat{\xi}_0^+ \neq \hat{\xi}_0^-$, this implies that the vector (t_I, t'_I) must obey

$$R^\mu = S^\mu = 0 \tag{3.62}$$

We can simplify the expression for R^μ as follows. Equating coefficients of different powers of ξ_0 in (3.19) gives

$$A_\star^{\mu 0\rho\sigma} = 0 \qquad \xi_i A_\star^{\mu i\rho\sigma} + B_\star^{\mu 0\rho\sigma} = 0 \qquad \xi_i B_\star^{\mu i\rho\sigma} + C_\star^{\mu 0\rho\sigma} = 0 \qquad \xi_i C_\star^{\mu i\rho\sigma} = 0 \tag{3.63}$$

It follows that R^μ depends only on the gauge-fixing term $\mathcal{P}_{\rm GF}$. A calculation now gives

$$R^\mu = -\frac{1}{2}\hat{g}^{00}g^{\mu\beta}\left(\tilde{P}_\beta{}^{i\rho\sigma}\xi_i t_{\rho\sigma} + \tilde{P}_\beta{}^{0\rho\sigma}t'_{\rho\sigma}\right) \tag{3.64}$$

and so $R^\mu = 0$ implies

$$\tilde{P}_\beta{}^{i\rho\sigma}\xi_i t_{\rho\sigma} + \tilde{P}_\beta{}^{0\rho\sigma}t'_{\rho\sigma} = 0 \tag{3.65}$$

(As a check, note that this equation is satisfied by the *eigenvectors* in $V^\pm$ and $\tilde{V}^\pm$ since these have $t'_{\rho\sigma} = \xi_0 t_{\rho\sigma}$, where ξ_0 is the eigenvalue and $t_{\mu\nu}$ satisfies (3.51).) Using this result, one can show that the gauge-fixing terms cancel out in S^μ. However we will not need to consider S^μ.

We have shown that any vector in $V^\pm$ or $\tilde{V}^\pm$ must satisfy (3.65). Consider now the possibility that $M(\xi_i)$ is *not* diagonalizable in V^+, which means that there is a non-trivial Jordan block associated to an eigenvalue ξ_0 belonging to the ξ_0^+ group. This implies that there is a vector $w \in V^+$ such that $(M(\xi_i) - \xi_0)^2 w = 0$ but $(M(\xi_i) - \xi_0)w \neq 0$. Hence $(M(\xi_i) - \xi_0)w$ is an eigenvector (in V^+) with eigenvalue ξ_0. Writing $w = (u_I, u'_I)^T$ this means

$$(M(\xi_i) - \xi_0)\begin{pmatrix} u \\ u' \end{pmatrix} = \begin{pmatrix} t \\ \xi_0 t \end{pmatrix} \tag{3.66}$$

for some $t_{\mu\nu}$ satisfying the characteristic condition (3.18) and the defining condition of case (i)

$$\tilde{P}_\alpha{}^{\gamma\rho\sigma}\xi_\gamma t_{\rho\sigma} = 0 \tag{3.67}$$

Writing out the components of (3.66) gives

$$u'_{\mu\nu} = \xi_0 u_{\mu\nu} + t_{\mu\nu} \tag{3.68}$$

and

$$\mathcal{P}(\xi)^{\mu\nu\rho\sigma}u_{\rho\sigma} = -(2\xi_0 A + B)^{\mu\nu\rho\sigma}t_{\rho\sigma} \tag{3.69}$$

Since the vector (u_I, u'_I) belongs to V^+, it must satisfy the constraint (3.65). This gives

$$\tilde{P}_\beta{}^{\gamma\rho\sigma}\xi_\gamma u_{\rho\sigma} + \tilde{P}_\beta{}^{0\rho\sigma}t_{\rho\sigma} = 0 \tag{3.70}$$

Now write (3.69) as

$$\mathcal{P}_\star(\xi)u = -\mathcal{P}_{\rm GF}(\xi)u - (2\xi_0 A_{\rm GF} + B_{\rm GF})t - (2\xi_0 A_\star + B_\star)t. \tag{3.71}$$

Using (3.70) and (3.67) we find that

$$\begin{aligned} -\left[\mathcal{P}_{\rm GF}(\xi)u + (2\xi_0 A_{\rm GF} + B_{\rm GF})t\right]^{\mu\nu} &= \hat{P}_\alpha{}^{\delta\mu\nu}\xi_\delta\tilde{P}^{\alpha\gamma\rho\sigma}\xi_\gamma u_{\rho\sigma} + \hat{P}_\alpha{}^{\delta\mu\nu}\xi_\delta\tilde{P}^{\alpha 0\rho\sigma}t_{\rho\sigma} \\ &\quad + \hat{P}_\alpha{}^{0\mu\nu}\tilde{P}^{\alpha\gamma\rho\sigma}\xi_\gamma t_{\rho\sigma} \\ &= \hat{P}_\alpha{}^{0\mu\nu}\tilde{P}^{\alpha\gamma\rho\sigma}\xi_\gamma t_{\rho\sigma} = 0, \end{aligned} \tag{3.72}$$

i.e. the gauge-fixing terms all cancel on the RHS of (3.71), leaving

$$\mathcal{P}_\star(\xi)^{\mu\nu\rho\sigma}u_{\rho\sigma} = -(2\xi_0 A_\star + B_\star)^{\mu\nu\rho\sigma}t_{\rho\sigma}. \tag{3.73}$$

Now contract this equation with $t^*_{\mu\nu}$ (the complex conjugate of $t_{\mu\nu}$). Since $\mathcal{P}_\star$ is symmetric we can write the LHS as $u\mathcal{P}_\star(\xi)t^*$ and this vanishes because $P_\star(\xi)t^* = (P_\star(\xi)t)^* = (P(\xi)t)^* = 0$ using the fact that t satisfies (3.67). So we are left with

$$0 = t^*_{\mu\nu}(2\xi_0 A_\star + B_\star)^{\mu\nu\rho\sigma}t_{\rho\sigma} = (v,v)_+ \tag{3.74}$$

where $v = (t_I, \xi_0 t_I)$ is the eigenvector. But we showed earlier that $(,)_+$ is positive definite. So we must have $v = 0$, which is a contradiction. Hence our assumption that there exists a non-trivial Jordan block must be false. Therefore $M(\xi_i)$ must be diagonalizable within V^+. A similar argument demonstrates that $M(\xi_i)$ is diagonalizable within V^-.

We have now proved that $M(\xi_i)$ is diagonalizable with real eigenvalues. Since $M(\xi_i)$ is real, this implies that we can choose the eigenvectors to be real. Our final task is to construct a symmetrizer. Note that the eigenvalues associated to $V^\pm$ are generically distinct and have non-trivial dependence on the Riemann tensor and ξ_i [59]. However, as ξ_i is varied, the eigenvalues might cross and if this happens then the eigenvectors might not be smooth functions of ξ_i [94]. This means that the standard choice of a symmetrizer in the subspaces $V^\pm$ might not be smooth in ξ_i, so the definition of strong hyperbolicity would not be satisfied. However, one can easily overcome this difficulty. Given two eigenvectors $v^{(1)}$ and $v^{(2)}$ in $V^\pm$ with respective eigenvalues $\xi_0^{(1)}$ and $\xi_0^{(2)}$ we have

$$v^{(1)T}\left(M^T H_\star^\pm - H_\star^\pm M\right)v^{(2)} = \left(\xi_0^{(1)} - \xi_0^{(2)}\right)v^{(1)T} H_\star^\pm v^{(2)} = 0 \tag{3.75}$$

where the final equality is (3.52). Since the eigenvectors form a basis for $V^\pm$, it follows that $H_\star^\pm$ is a symmetrizer for $M(\xi_i)$ within $V^\pm$. Crucially, $H_\star^\pm$ depends smoothly on ξ_i. We now construct a symmetrizer for $M(\xi_i)$ within V as a block diagonal matrix where the blocks associated to $\tilde{V}^\pm$ and $\hat{V}^\pm$ are constructed from the (smooth) eigenvectors in the usual way, and the blocks associated to $V^\pm$ are equal to $H_\star^\pm$. More explicitly, let $\{v_1^\pm, ..., v_{d(d-3)/2}^\pm\}$ be a smooth basis for $V^\pm$ and let $\{\tilde{v}_1^\pm, ..., \tilde{v}_d^\pm\}$ and $\{\hat{v}_1^\pm, ..., \hat{v}_d^\pm\}$ denote the smooth eigenvectors (constructed above) in $\tilde{V}^\pm$ and $\hat{V}^\pm$ respectively. Furthermore, let S be the matrix whose columns are these (real) basis vectors. Then $M(\xi_i)$ can be written as

$$M(\xi_i) = S\begin{pmatrix} \Xi^+ & 0 & 0 & 0 & 0 & 0 \\ 0 & \tilde{\xi}_0^+ I_d & 0 & 0 & 0 & 0 \\ 0 & 0 & \hat{\xi}_0^+ I_d & 0 & 0 & 0 \\ 0 & 0 & 0 & \Xi^- & 0 & 0 \\ 0 & 0 & 0 & 0 & \tilde{\xi}_0^- I_d & 0 \\ 0 & 0 & 0 & 0 & 0 & \hat{\xi}_0^- I_d \end{pmatrix} S^{-1} \tag{3.76}$$

where $\Xi^{\pm}$ are $d(d-3)/2 \times d(d-3)/2$ matrices and I_d is the $d \times d$ unit matrix. Our proposal for the symmetrizer can also be written in a decomposed form as

$$K(\xi_i) = \left(S^{-1}\right)^T \begin{pmatrix} \mathcal{H}_\star^+ & 0 & 0 & 0 & 0 & 0 \\ 0 & I_d & 0 & 0 & 0 & 0 \\ 0 & 0 & I_d & 0 & 0 & 0 \\ 0 & 0 & 0 & \mathcal{H}_\star^- & 0 & 0 \\ 0 & 0 & 0 & 0 & I_d & 0 \\ 0 & 0 & 0 & 0 & 0 & I_d \end{pmatrix} S^{-1} \tag{3.77}$$

where $\mathcal{H}_\star^{\pm}$ are the $d(d-3)/2 \times d(d-3)/2$ matrices whose elements are $(\hat{A}, \hat{B} = 1, 2, ..., d(d-3)/2)$

$$\left(\mathcal{H}_\star^{\pm}\right)_{\hat{A}\hat{B}} = \left(v_{\hat{A}}^{\pm}\right)^T H_\star^{\pm} v_{\hat{B}}^{\pm} \tag{3.78}$$

The matrix given by (3.77) then clearly satisfies (3.17) and therefore it is indeed a symmetrizer. Moreover, as explained above, it depends smoothly on ξ_i. This concludes the proof of strong hyperbolicity.

3.4 Horndeski theories

In this section, we will analyze the hyperbolicity of the equations of motion of weakly coupled Horndeski theories in modified harmonic gauge. Our discussion uses similar ideas to the Lovelock case so to avoid repetition, we will merely point out the differences.

3.4.1 Principal symbol

The action for a general Horndeski theory is given by (1.9). As mentioned, we could absorb the terms in $\mathcal{L}_1$ into other terms; the reason we do not do this is that we want to regard a weakly coupled Horndeski theory as a small deformation of GR.

Variation of (1.9) w.r.t. the metric and scalar field yields the equations of motion

$$E^{\mu\nu} \equiv -16\pi G \frac{1}{\sqrt{-g}} \frac{\delta S}{\delta g_{\mu\nu}} = 0, \qquad E_\phi \equiv -16\pi G \frac{1}{\sqrt{-g}} \frac{\delta S}{\delta \phi} = 0 \tag{3.79}$$

The explicit form of these equations for the most general Horndeski theory can be found in e.g. Appendix A of [61].

Our modified harmonic gauge equations of motion are defined in exactly the same way as in GR and for Lovelock theories. We introduce the two auxiliary (inverse) metrics $\tilde{g}^{\mu\nu}$ and $\hat{g}^{\mu\nu}$ satisfying the same conditions as in section 3.2.1. The gravitational equation of motion is modified as in equation (3.5) and the scalar equation is left unchanged, so the equations of motion are

$$E^{\mu\nu}_{\mathrm{mhg}} \equiv E^{\mu\nu} + \hat{P}_{\alpha}{}^{\beta\mu\nu}\partial_\beta H^\alpha = 0 \tag{3.80}$$

and

$$E_\phi = 0. \tag{3.81}$$

Initial data for Horndeski theories consists of a quintuple $(\Sigma, h_{\mu\nu}, K_{\mu\nu}, \Phi, \Psi)$ where $h_{\mu\nu}$ and $K_{\mu\nu}$ correspond to the induced metric and extrinsic curvature tensor of Σ, and Φ, Ψ to the values of ϕ and its normal derivative on Σ. The equations $E^{\mu\nu}n_\nu = 0$ contain no second time derivatives of ϕ and g so they are constraint equations that the initial data must satisfy.

The diffeomorphism invariance of the action implies that, for any $g_{\mu\nu}$ and ϕ, we have the generalized Bianchi identity

$$\nabla^\mu E_{\mu\nu} - E_\phi \nabla_\nu \phi = 0. \tag{3.82}$$

Since there are no gauge fixing terms in the scalar equation of motion, this identity implies that the equation describing the propagation of the gauge condition H^μ remains the same as in GR, i.e., the deformed harmonic gauge equations of motion implies that H^μ satisfies (3.8). Thus if H^μ and its normal derivative vanish on Σ then H^μ will vanish throughout $\hat{D}(\Sigma)$, as in section 3.2.2.

To construct initial data for (3.80), (3.81) we proceed as in section 3.2.2, writing the metric in terms of the lapse and shift to ensure that the surface $x^0 = 0$ is spacelike w.r.t. $g^{\mu\nu}$. The time derivative of the lapse and shift are chosen to ensure that $H^\mu = 0$ at $x^0 = 0$ and the constraint equations then imply that the derivative of H^μ vanishes at $x^0 = 0$ as in section 3.2.2. Hence H^μ vanishes throughout $\hat{D}(\Sigma)$ and so the resulting solution of (3.80) and (3.81) is also a solution of the original Horndeski equations of motion in $\hat{D}(\Sigma)$ and hence also in $D(\Sigma)$.

A general Horndeski theory is not quasilinear. We define the principal symbol by varying the equation of motion w.r.t. the second derivatives of the fields, as explained in section 1.2. The principal symbol acts on a vector of the form $T_I \equiv (t_{\mu\nu}, \psi)^T$ where $t_{\mu\nu}$ is symmetric. The space of such vectors is 11-dimensional so indices $I, J, \ldots$ take values from 1 to 11. We label the different blocks of the principal symbol as follows:

$$\mathcal{P}(\xi)^{IJ} = \mathcal{P}^{IJ\gamma\delta}\xi_\gamma\xi_\delta = \begin{pmatrix} \mathcal{P}_{gg}(\xi)^{\mu\nu\rho\sigma} & \mathcal{P}_{g\phi}(\xi)^{\mu\nu} \\ \mathcal{P}_{\phi g}(\xi)^{\rho\sigma} & \mathcal{P}_{\phi\phi}(\xi) \end{pmatrix}. \tag{3.83}$$

In other words:

$$\mathcal{P}(\xi)^{IJ}T_J = \begin{pmatrix} \mathcal{P}_{gg}(\xi)^{\mu\nu\rho\sigma}t_{\rho\sigma} + \mathcal{P}_{g\phi}(\xi)^{\mu\nu}\psi \\ \mathcal{P}_{\phi g}(\xi)^{\rho\sigma}t_{\rho\sigma} + \mathcal{P}_{\phi\phi}(\xi)\psi \end{pmatrix}. \tag{3.84}$$

We decompose the principal symbol as in (3.9) into a part $\mathcal{P}_\star$ coming from (3.79) and a part $\mathcal{P}_{\rm GF}$ coming from the gauge fixing term. The former can be written

$$\mathcal{P}_\star(\xi)^{IJ} = \begin{pmatrix} \mathcal{P}_{gg\star}(\xi)^{\mu\nu\rho\sigma} & \mathcal{P}_{g\phi\star}(\xi)^{\mu\nu} \\ \mathcal{P}_{\phi g\star}(\xi)^{\rho\sigma} & \mathcal{P}_{\phi\phi\star}(\xi) \end{pmatrix}. \tag{3.85}$$

where the 11×11 matrix $\mathcal{P}_\star(\xi)^{IJ}$ is *symmetric* because the equations of motion (without gauge-fixing) are obtained from an action [60]. In particular we have

$$\mathcal{P}_{g\phi\star}(\xi)^{\mu\nu} = \mathcal{P}_{\phi g\star}(\xi)^{\mu\nu} \tag{3.86}$$

The contribution of the gauge-fixing term to the principal symbol is

$$\mathcal{P}_{\rm GF}(\xi)^{IJ} = \begin{pmatrix} -\hat{P}_\alpha{}^{\gamma\mu\nu}\xi_\gamma g^{\alpha\beta}\tilde{P}_\beta{}^{\delta\rho\sigma}\xi_\delta & 0 \\ 0 & 0 \end{pmatrix} \tag{3.87}$$

It is useful to split $\mathcal{P}_\star$ into the sum of two terms corresponding to the contributions from the Einstein-scalar field Lagrangian $\mathcal{L}_1$ and the Horndeski terms $\mathcal{L}_i$ with $i \geq 2$ respectively:

$$\mathcal{P}_\star(\xi)^{IJ} = \mathcal{P}_\star^{\rm Esf}(\xi)^{IJ} + \delta\mathcal{P}_\star(\xi)^{IJ} \tag{3.88}$$

where the Einstein-scalar-field part is

$$\mathcal{P}_\star^{\rm Esf}(\xi)^{IJ} = \begin{pmatrix} -\frac{1}{2}g^{\gamma\delta}\xi_\gamma\xi_\delta P^{\mu\nu\rho\sigma} + P_\alpha{}^{\gamma\mu\nu}\xi_\gamma g^{\alpha\beta}P_\beta{}^{\delta\rho\sigma}\xi_\delta & 0 \\ 0 & -g^{\gamma\delta}\xi_\gamma\xi_\delta \end{pmatrix}. \tag{3.89}$$

The form of the Horndeski terms $\delta\mathcal{P}_\star(\xi)^{IJ}$ can be found in Appendix B of [61]. As in the case of Lovelock theories, we define "weak coupling" to mean that $\delta\mathcal{P}_\star(\xi)^{IJ}$ is small compared to $\mathcal{P}_\star^{\rm Esf}(\xi)^{IJ}$. This will be the case if the Riemann tensor and first and second derivatives of the scalar field are small compared to any length scales defined by the (dimensionful) Horndeski coupling functions $G_i(\phi, X)$ and their derivatives w.r.t. X. As in the Lovelock case, if the initial data is chosen so that the theory is weakly coupled initially then, by continuity, the resulting solution will remain weakly coupled at least for a small time. But the theory may become strongly coupled over a longer time, in which case even weak hyperbolicity of the equations of motion may fail [60, 62–64].

The equations of motion of a generic Horndeski theory are not quasilinear but they have the same special structure as Lovelock theories, i.e., in any chart, they are linear in second derivatives w.r.t. any given coordinate[5], and this property is not affected by the gauge fixing term. Hence, in a chart $x^\mu = (x^0, x^i)$, the modified harmonic gauge equation of motion can be written as

$$A^{IJ}(x, u, \partial_\mu u, \partial_0\partial_i u, \partial_i\partial_j u)\partial_0^2 u_J = F^I(x, u, \partial_\mu u, \partial_0\partial_i u, \partial_i\partial_j u) \tag{3.90}$$

with $u_I = (g_{\mu\nu}, \phi)$ and A^{IJ} is defined in terms of $\mathcal{P}^{IJ}$ as in (3.15). So the equations are linear in the second time derivatives of the fields. In Einstein-scalar-field theory, the matrix A^{IJ} is invertible on surfaces of constant x^0 provided such surfaces are spacelike, i.e., spacelike surfaces are non-characteristic. By continuity, a spacelike hypersurface remain non-characteristic for a sufficiently weakly coupled Horndeski theory. Therefore, if we can show that the system (3.80)-(3.81) is strongly hyperbolic then the results reviewed in section 1.2 will apply and local well-posedness of the initial value problem for weakly coupled Horndeski theories would be established.

3.4.2 Proof of strong hyperbolicity

Using a coordinate system $x^\mu = (x^0, x^i)$, the 11×11 matrices A^{IJ}, B^{IJ}, C^{IJ} are defined by (3.15). To analyze the hyperbolicity of the equations of motion (3.80)-(3.81), we must study the eigenvalue problem of the 22×22 matrix $M(\xi_i)$ defined by equation (3.16), where ξ_i is a real covector with unit norm w.r.t. an arbitrary smooth (inverse) Riemannian metric G^{ij} defined on surfaces of constant x^0. This matrix acts on the 22-dimensional vector space V of complex vectors of the form $v = (T_I, T'_I)^T$ with $T_I = (t_{\mu\nu}, \psi)^T$, $T'_I = (t'_{\mu\nu}, \psi')^T$. An eigenvector corresponding to an eigenvalue ξ_0 has

[5] This can be seen from the equations of motion written out in Appendix A of Ref. [61]. Second derivatives w.r.t. x^α appear only in the Riemann tensor component $R_{\alpha\mu\alpha\nu}$ (or components related by antisymmetry) and in $\nabla_\alpha\nabla_\alpha\phi$. Non-quasilinear terms all have antisymmetrizations which prevent two indices c_i (in the equations of [61]) being equal to α and hence products of second derivative w.r.t. x^α do not appear.

the form $(T_I, \xi_0 T_I)^T$ where T_I satisfies

$$\mathcal{P}(\xi)^{IJ} T_J = 0 \tag{3.91}$$

with $\xi_\mu = (\xi_0, \xi_i)$, i.e., ξ_μ is characteristic with associated "polarization" T_I.

We start by considering Einstein-scalar field theory. If ξ_0 is an eigenvalue for vacuum GR, with eigenvector $(t_{\mu\nu}, \xi_0 t_{\mu\nu})^T$ then ξ_0 is also an eigenvalue for Einstein-scalar-field theory with eigenvector $(T_I, \xi_0 T_I)^T$ where $T_I = (t_{\mu\nu}, 0)^T$ (i.e. T_I has $\psi = 0$). This gives us "pure gauge" eigenvalues $\tilde{\xi}_0^{\pm}$ and "gauge-condition violating" eigenvalues $\hat{\xi}_0^{\pm}$, each with 4 eigenvectors, and "physical" eigenvalues $\xi_0^{\pm}$, each with 2 eigenvectors. A further physical eigenvector with eigenvalue $\xi_0^{\pm}$ is obtained by setting $t_{\mu\nu} = 0$ and $\psi = 1$. Thus for each physical eigenvalue $\xi_0^{\pm}$ there are 3 eigenvectors, corresponding to 2 graviton polarizations and 1 scalar field polarization. The eigenvalues are all real, the total number of eigenvectors is 22, and the eigenvectors depend smoothly on ξ_i. Hence our modified harmonic gauge formulation of Einstein-scalar field theory is strongly hyperbolic.

Now we consider a weakly coupled Horndeski theory. Just as for a weakly coupled Lovelock theory, continuity of the eigenvalues implies that the eigenvalues of $M(\xi_i)$ for weakly coupled Horndeski theories can be split into 6 groups. The decomposition

$$V = V^+ \oplus \tilde{V}^+ \oplus \hat{V}^+ \oplus V^- \oplus \tilde{V}^- \oplus \hat{V}^- \tag{3.92}$$

into total generalized eigenspaces and the definition of the corresponding projection matrices (3.46) (that depend smoothly on ξ_i, the background fields and the Horndeski couplings) is the same as for the Lovelock case. The counting of eigenvectors for Einstein-scalar field theory implies that the spaces $\tilde{V}^{\pm}$ and $\hat{V}^{\pm}$ are 4-dimensional whereas $V^{\pm}$ are 3-dimensional.

Analogously to equation (3.19), diffeomorphism invariance of the action implies that [60]

$$\mathcal{P}_{gg\star}(\xi)^{\mu\nu\rho\sigma} \xi_\nu = 0, \qquad \mathcal{P}_{g\phi\star}(\xi)^{\mu\nu} \xi_\nu = 0. \tag{3.93}$$

The characteristic equation is (3.91). Writing the LHS as in (3.84), taking the contraction of the first row with ξ_ν, and using (3.93), we obtain equation (3.20). Hence the analysis splits into case (i) and case (ii) just as for vacuum GR and for Lovelock theories. For Einstein-scalar field theory we can split case (i) into subcases (ia) and (ib), as in GR, where the physical eigenvectors with $t_{\mu\nu} = 0$ are included in subcase (ib).

In Einstein-scalar field theory, subcase (ia) gives the "pure gauge" eigenvectors with eigenvalues $\tilde{\xi}_0^{\pm}$ and $T_I = (\tilde{\xi}^{\pm}_{(\mu} X_{\nu)}, 0)^T$ for any X_ν. These are also eigenvectors for a Horndeski theory, with the same (real) eigenvalues $\tilde{\xi}_0^{\pm}$. So the spaces $\tilde{V}^{\pm}$ are genuine eigenspaces spanned by these eigenvectors. In Einstein-scalar field theory, subcase (ib) gives the "physical" eigenvectors with eigenvalues $\xi_0^{\pm}$. We will discuss the Horndeski generalization of these below.

Case (ii) is defined by (3.31), so the (real) eigenvalues are $\hat{\xi}_0^{\pm}$ as in Einstein-scalar field theory. The corresponding "gauge condition violating" eigenvectors can be constructed similarly to the Lovelock case. One can introduce a smooth orthonormal (w.r.t. $g_{\mu\nu}$) basis adapted to $\hat{\xi}^{\pm}_\mu$ (see the paragraphs above (3.32)) with indices $A, B \ldots$ labelling directions orthogonal to $\hat{\xi}^{\pm}_\mu$, which is spacelike w.r.t. $g^{\mu\nu}$. Equation (3.93) implies that the only non-vanishing components of $\mathcal{P}_{gg\star}(\hat{\xi}^{\pm})^{\mu\nu\rho\sigma}$ and $\mathcal{P}_{g\phi\star}(\hat{\xi}^{\pm})^{\mu\nu}$ are the $ABCD$ and AB components respectively.

We then fix a vector v^μ and consider the equation

$$\begin{pmatrix} \mathcal{P}_{gg\star}(\hat{\xi}^{\pm})^{ABCD} & \mathcal{P}_{g\phi\star}(\hat{\xi}^{\pm})^{AB} \\ \mathcal{P}_{\phi g\star}(\hat{\xi}^{\pm})^{CD} & \mathcal{P}_{\phi\phi\star}(\hat{\xi}^{\pm}) \end{pmatrix} \begin{pmatrix} t_{CD} \\ \psi \end{pmatrix} = \begin{pmatrix} \hat{P}_\alpha{}^{\beta AB} \hat{\xi}^{\pm}_\beta v^\alpha \\ 0 \end{pmatrix} \tag{3.94}$$

We will show that the matrix on the LHS is invertible in a weakly coupled Horndeski theory. Consider first the case of Einstein-scalar field theory. In this case, the matrix on the LHS is block diagonal and (s_{AB}, χ) belongs to the kernel iff

$$\begin{aligned} \mathcal{P}_{gg\star}(\hat{\xi}^{\pm})^{ABCD} s_{CD} &= 0 \\ g^{\gamma\delta} \hat{\xi}^{\pm}_\gamma \hat{\xi}^{\pm}_\delta \chi = 0. \end{aligned} \tag{3.95}$$

Since $g^{\gamma\delta} \hat{\xi}^{\pm}_\gamma \hat{\xi}^{\pm}_\delta \neq 0$, we have $\chi = 0$ and the argument used in the vacuum GR case establishes that $s_{AB} = 0$, so the kernel is trivial in Einstein-scalar field theory. Thus the matrix on the LHS of (3.94) has non-vanishing determinant in Einstein-scalar field theory. By continuity, its determinant must be non-zero for a weakly coupled Horndeski theory. Hence this matrix is invertible. So, for each v^μ, this equation uniquely defines $(t_{AB}(v), \psi(v))$. This will depend smoothly on v^μ. It also depends smoothly on ξ_i because the matrix on the LHS, and the RHS of (3.94) depend smoothly on ξ_i.

The rest of the argument proceeds as in GR: define $X_\mu(v)$ as in (3.39) and $t_{\mu\nu}(v)$ as in (3.40). Let $T_I(v) = (t_{\mu\nu}(v), \psi(v))^T$. We then have $\mathcal{P}^{IJ}(\hat{\xi}^\pm)T_J(v) = 0$. Thus for each v^μ we have constructed an eigenvector. Letting v^μ run over a basis of 4 linearly independent vectors gives us 4 linearly independent eigenvectors. Thus we have proved that $\hat{V}^\pm$ are genuine eigenspaces. The eigenvectors depend smoothly on ξ_i.

It remains to show that the physical spaces $V^\pm$ are genuine eigenspaces. Following the argument we used for Lovelock theories, we define the matrix $H_\star$ by equation (3.47) and the corresponding Hermitian form on $V^\pm$ by (3.48). In Einstein-scalar field theory, $V^\pm$ are genuine eigenspaces (this is subcase (ib)) and we can use the null basis introduced above equation (3.28) to show that this Hermitian form is

$$(v^{(1)}, v^{(2)})_\pm = \mp\xi^{\pm 0}\left(t^{(1)*}_{\hat{i}\hat{j}} t^{(2)}_{\hat{i}\hat{j}} + 2\psi^*\psi\right). \tag{3.96}$$

This is positive definite. By continuity, it remains positive definite for a weakly coupled Horndeski theory. Hence we have shown that our Hermitian form defines an inner product on $V^\pm$.

Just as for a Lovelock theory, the defining equation of case (i), i.e. (3.51), and the symmetry of $\mathcal{P}_\star$ imply the identity

$$\left(\xi_0^{(1)} - \xi_0^{(2)}\right) v^{(1)T} H_\star^+ v^{(2)} = 0 \tag{3.97}$$

(c.f. (3.52)) for two eigenvectors $v^{(1)} = (T^{(1)}, \xi_0^{(1)} T^{(1)})^T$ and $v^{(2)} = (T^{(2)}, \xi_0^{(2)} T^{(2)})^T$ belonging to $V^\pm$ with respective eigenvalues $\xi_0^{(1)}$ and $\xi_0^{(2)}$. We then follow the argument used for Lovelock theory to conclude that positive definiteness of the inner product on $V^\pm$ ensures that the eigenvalues in the $\xi_0^\pm$-groups are real, as in a weakly coupled Lovelock theory.

The final step is to show that $M(\xi_i)$ is diagonalizable on $V^\pm$. Again we follow the argument used for Lovelock theories and consider the left eigenvectors of $M(\xi_i)$. The left eigenvectors corresponding to the eigenvalue $\hat{\xi}_0^\pm$ have the form (3.54) where $s_I = (\hat{\xi}^\pm_{(\mu} X_{\nu)}, 0)^T$, for arbitrary X_μ. From the Jordan decomposition of $M(\xi_i)$, the subspaces V^+, V^-, $\tilde{V}^+$ and $\tilde{V}^-$ must be orthogonal to these eigenvectors for any X_μ and both choices of sign in $\hat{\xi}^\pm_\mu$. For $v = (T_I, T'_I)^T$ in one of these subspaces, this implies that[6]

$$R^\mu \equiv -2\left(\hat{g}^{00}\right)^{-1}\hat{g}^{0i}\xi_i A^{\mu 0J}T_J + B^{\mu 0J}T_J + \xi_i A^{\mu iJ}T_J + A^{\mu 0J}T'_J = 0 \tag{3.98}$$

and

$$S^\mu \equiv -\left(\hat{g}^{00}\right)^{-1}\hat{g}^{ij}\xi_i\xi_j A^{\mu 0J}T_J + \xi_i B^{\mu iJ}T_J + \xi_i A^{\mu iJ}T'_J = 0 \tag{3.99}$$

Similarly to the Lovelock case, writing out equation (3.93) in terms of the coefficients $A_\star^{IJ}$, $B_\star^{IJ}$ and $C_\star^{IJ}$ gives

$$A_\star^{\mu 0I} = 0 \qquad \xi_i A_\star^{\mu iI} + B_\star^{\mu 0I} = 0 \qquad \xi_i B_\star^{\mu iI} + C_\star^{\mu 0I} = 0 \qquad \xi_i C_\star^{\mu iI} = 0 \tag{3.100}$$

This implies that R^μ depends only on the principal symbol of the gauge-fixing terms, given in (3.87). Writing $T_I = (t_{\mu\nu}, \psi)^T$ and $T'_I = (t'_{\mu\nu}, \psi')^T$, the expression for R^μ reduces to

$$R^\mu = -\frac{1}{2}\hat{g}^{00}g^{\mu\beta}\left(\tilde{P}_\beta{}^{i\rho\sigma}\xi_i t_{\rho\sigma} + \tilde{P}_\beta{}^{0\rho\sigma}t'_{\rho\sigma}\right). \tag{3.101}$$

Therefore any vector in $V^\pm$ (or $\tilde{V}^\pm$) must satisfy

$$\tilde{P}_\beta{}^{i\rho\sigma}\xi_i t_{\rho\sigma} + \tilde{P}_\beta{}^{0\rho\sigma}t'_{\rho\sigma} = 0. \tag{3.102}$$

The proof of the diagonalizability of $M(\xi_i)$ in $V^\pm$ is the same as for a weakly coupled Lovelock theory. Assume that there exists a non-trivial Jordan block in V^+ with corresponding eigenvalue ξ_0. Then there must be a vector $w \equiv (U_I, U'_I)^T \in V^+$ such that $(M(\xi_i) - \xi_0)w \neq 0$ is an eigenvector $v \equiv (T_I, \xi_0 T_I) \in V^+$ with eigenvalue ξ_0. This is equivalent to the equations

$$U'_I = \xi_0 U_I + T_I \tag{3.103}$$

and

$$\mathcal{P}(\xi)^{IJ}U_J = -(2\xi_0 A + B)^{IJ}T_J. \tag{3.104}$$

where T_I satisfies (3.91) and if we write $T_I = (t_{\mu\nu}, \psi)$ then $t_{\mu\nu}$ satisfies (3.21) (the defining condition of case (i)).

Decomposing (3.104) into the contributions of $\mathcal{P}_\star$ and $\mathcal{P}_{\mathrm{GF}}$ as in (3.71), it can be shown that the gauge fixing terms cancel each other out. To see this, we note that the vector $w \equiv (U_I, U'_I)$ lies in V^+ so it is subject to the constraint (3.102). Since the only nonzero

[6] Recall that indices $I, J, \ldots$ label vectors of the form $T_I = (t_{\mu\nu}, \psi)^T$ where $t_{\mu\nu}$ is symmetric. $A^{\mu 0J}$ means the $I = (\mu 0)$ component of A^{IJ}, i.e., the component corresponding to $t_{\mu 0}$.

components of $\mathcal{P}_{\mathrm{GF}}$ are $\mathcal{P}_{\mathrm{GF}}(\xi)^{\mu\nu\rho\sigma}$, a calculation identical to (3.72) establishes

$$\mathcal{P}_{\mathrm{GF}}(\xi)^{IJ}U_J = -(2\xi_0 A_{\mathrm{GF}} + B_{\mathrm{GF}})^{IJ}T_J. \tag{3.105}$$

Contraction of the remaining terms in (3.104) with T_I^* gives

$$T_I^* \mathcal{P}_\star(\xi)^{IJ}U_J = -T_I^*(2\xi_0 A_\star + B_\star)^{IJ}T_J = (v, v)_+. \tag{3.106}$$

The symmetry of $\mathcal{P}_\star$ implies that the LHS can be written as $U\mathcal{P}_\star T^* = U(\mathcal{P}_\star T)^*$, which vanishes because $\mathcal{P}_\star T = \mathcal{P}T = 0$ using the fact that $t_{\mu\nu}$ obeys (3.21) and T_I obeys (3.91). Since the inner product on the RHS of (3.106) is positive definite, it follows that $v = 0$, which is a contradiction. Hence, $M(\xi_i)$ does not admit a non-trivial Jordan block in V^+, i.e., $M(\xi_i)$ is diagonalizable in V^+. The diagonalizability of $M(\xi_i)$ in V^- follows similarly.

Since $M(\xi_i)$ has a basis of eigenvectors on the spaces $V^\pm$, it follows from the identity (3.97) that $H_\star$ is a symmetrizer on $V^\pm$. The definition of $H_\star$ shows that this symmetrizer is a smooth function of ξ_i (even if the eigenvectors are not[7]). A symmetrizer on V is now constructed from the (smooth) eigenvectors on $\tilde{V}^\pm$ and $\hat{V}^\pm$ and the (smooth) inner product $H_\star$ on $V^\pm$, just as for a weakly coupled Lovelock theory.

This concludes the proof of strong hyperbolicity for weakly coupled Horndeski theories.

3.5 Discussion

3.5.1 Application to numerical relativity

Our modified harmonic gauge equations of motion involve two auxiliary Lorentzian inverse metrics $\tilde{g}^{\mu\nu}$ and $\hat{g}^{\mu\nu}$ as well as the physical inverse metric $g^{\mu\nu}$. The only conditions that we have imposed on these inverse metrics is that their causal cones should form a nested set as in Fig. 3.1. Our reasons for imposing these restrictions on the null cones are threefold: (i) we can ensure that our initial surface is spacelike w.r.t. all three metrics simultaneously; (ii) our proof of strong hyperbolicity of the gauge fixed equations requires that the null cones of the three metrics do not intersect; (iii) in GR our assumption that $g^{\mu\nu}$ has the innermost null cone (in the cotangent space), and hence $g_{\mu\nu}$ has the outermost null cone (in the tangent space), implies that the

[7]As for a Lovelock theory, the physical eigenvectors may exhibit non-smoothness as a function of ξ_i at values of ξ_i for which two or more physical eigenvalues are degenerate.

causal properties of the gauge fixed equations of motion are determined by the physical metric rather than either of the auxiliary metrics.

Clearly there is considerable freedom in how we choose these metrics. A method that might be useful in numerical applications is as follows. Let n_μ be a unit (w.r.t. $g^{\mu\nu}$) normal to surfaces of constant x^0. We now choose

$$\tilde{g}^{\mu\nu} = g^{\mu\nu} - a n^\mu n^\nu \qquad \hat{g}^{\mu\nu} = g^{\mu\nu} - b n^\mu n^\nu. \tag{3.107}$$

Our assumptions about the causal cones of the three metrics require that the functions $a(x)$ and $b(x)$ satisfy

$$0 < a(x) < b(x) \qquad \text{or} \qquad 0 < b(x) < a(x). \tag{3.108}$$

This ensures that the null cones are nested either as in Fig. 3.1 or as in Fig. 3.1 with the null cones of $\tilde{g}^{\mu\nu}$ and $\hat{g}^{\mu\nu}$ interchanged. The simplest possibility would be to choose a and b to be constants satisfying the above inequalities.

Although requirement (iii) is natural, it may not be essential for numerical relativity simulations. If one is willing to give up (iii) then the ordering of the causal cones in Fig. 3.1 can be changed. If we interchange the null cones of $g^{\mu\nu}$ and $\tilde{g}^{\mu\nu}$ in Fig. 3.1 then we have the alternative condition

$$-1 < a(x) < 0 < b(x) \tag{3.109}$$

where the lower bound arises from the requirement that $\tilde{g}^{\mu\nu}$ is Lorentzian. In this case, causal properties of the gauge-fixed equation of motion will be determined by the unphysical metric $\tilde{g}^{\mu\nu}$, and we need to choose the initial lapse and shift to ensure that the initial surface is spacelike w.r.t. $\tilde{g}^{\mu\nu}$.

For a Lovelock or Horndeski theory, strong hyperbolicity requires that the physical characteristics do not intersect the null cones of $\tilde{g}^{\mu\nu}$ and $\hat{g}^{\mu\nu}$, which will be the case at sufficiently weak coupling for any a, b satisfying (3.108) or (3.109). For stronger fields, one would not want a failure of strong hyperbolicity to arise simply from having chosen the null cones of $\tilde{g}^{\mu\nu}$ and $\hat{g}^{\mu\nu}$ too close to the null cone of $g^{\mu\nu}$, so a, b should not be too close to zero. This should ensure that a failure of strong hyperbolicity (for stronger fields) arises from the behaviour of the physical degrees of freedom of the theory, rather than from the gauge fixing procedure. In a numerical simulation, one could check this by adjusting a, b to see whether this extends the time for which the simulation runs.

Our formulation may have some advantages even for conventional GR. In numerical relativity, it might be possible to tailor the choice of $\tilde{g}^{\mu\nu}$ and $\hat{g}^{\mu\nu}$ to one's needs. For example, consider the choice (3.107) with $a = \alpha/2 - 1$ where α is the lapse function. Note that (3.108) requires $2 < \alpha < 4$ whereas (3.109) allows $0 < \alpha < 2$. In this case, the $\mu = 0$ component of the modified harmonic gauge condition $H^\mu = 0$ gives the so-called $1 + \log$ slicing condition (where β^k is the shift vector, K is the trace of the extrinsic curvature $K_{ij} = -1/2\ \mathcal{L}_n h_{ij}$)

$$(\partial_t - \beta^k \partial_k)\alpha = -2K\alpha \tag{3.110}$$

This is a popular choice of slicing due to its good singularity avoidance properties (see e.g. [84] and the references therein).

As in conventional harmonic gauge, one has the option to introduce suitable source functions $F^\mu(x)$ and impose the generalized modified harmonic gauge condition

$$H^\mu \equiv -\tilde{g}^{\rho\sigma}\Gamma^\mu_{\rho\sigma} - F^\mu(x) = 0. \tag{3.111}$$

Finally, the growth of numerical errors may be dealt with in the usual way [89], i.e. by adding lower order homogeneous gauge fixing terms so that the equation of motion for the metric becomes

$$E^{\mu\nu} + \hat{P}_\alpha{}^{\beta\mu\nu}\partial_\beta H^\alpha - \kappa_1 \left(n^\mu H^\nu + n^\nu H^\mu + \kappa_2\ n^\alpha H_\alpha\ g^{\mu\nu}\right) = 0 \tag{3.112}$$

where the constants κ_1, κ_2 are chosen so that constraint violations are damped away during the evolution.

3.5.2 Domain of dependence

In a Lovelock or Horndeski theory, the "physical" characteristic covectors (i.e. those associated to $V^\pm$) are generically non-null w.r.t. $g^{\mu\nu}$, with some of them spacelike and others timelike. (Some explicit examples have been studied in [59].) This means that causal properties of the theory are not determined by the null cone of $g_{\mu\nu}$. We will now discuss, in qualitative terms, the implications of this for the domain of dependence properties of these theories. We assume that the causal cones of the three metrics are related as in Fig. 3.1.

Let (M, g) be a spacetime satisfying the modified harmonic gauge Lovelock or Horndeski equation(s) of motion and the weakly coupled assumption. Let $\Sigma \subset M$ be an initial data surface, i.e., Σ is spacelike w.r.t. $g^{\mu\nu}$ and is therefore non-characteristic (for sufficiently weak coupling, as explained above). Assume that the constraint equations and the harmonic gauge condition are satisfied on Σ. Then, as explained above, $g_{\mu\nu}$ will satisfy the original Lovelock/Horndeski equation(s) of motion in $\hat{D}(\Sigma) \subset M$.

Now let Ω be a connected open subset of Σ. We define the domain of dependence of Ω, denoted $\mathcal{D}(\Omega)$, to be the region of spacetime in which the solution does not change if we vary the initial data on $\Sigma \backslash \Omega$, keeping the data on Ω fixed. Strong hyperbolicity guarantees *local* well-posedness, which ensures that the solution is unique in a neighbourhood of Ω so $\mathcal{D}(\Omega)$ is non-empty. We define the Cauchy horizon of Ω, denoted $\mathcal{H}(\Omega)$ to be the boundary of $\mathcal{D}(\Omega)$ in M. This will have two components: the future and past Cauchy horizons $\mathcal{H}^{\pm}(\Omega)$. We expect these to be the "innermost ingoing" characteristic hypersurfaces of (3.42) emanating from, and tangential to, $\partial\Omega$, the boundary of Ω.[8]

In modified harmonic gauge GR (or Einstein-scalar field theory), there are three types of characteristic surface, namely surfaces that are null w.r.t. one of the three inverse metrics. The ordering of the null cones assumed in Fig. 3.1 implies that $D(\Omega) \subset \hat{D}(\Omega)$ and $D(\Omega) \subset \tilde{D}(\Omega)$, so it follows that the innermost ingoing characteristic hypersurface is null w.r.t. $g^{\mu\nu}$ and so $\mathcal{D}(\Omega) = D(\Omega)$, the domain of dependence defined w.r.t. the physical metric. So we have recovered the usual domain of dependence property of GR.

In a weakly coupled modified harmonic gauge Lovelock/Horndeski theory, a characteristic surface is either null w.r.t. $\hat{g}^{\mu\nu}$ or w.r.t. $\tilde{g}^{\mu\nu}$ or its normal covector is associated to an eigenvector belonging to the "physical" space $V^{\pm}$. Generically, we expect $N = (1/2)d(d-3)$ distinct eigenvectors in each of $V^{\pm}$ and so generically there will be N "physical" ingoing characteristic surfaces emanating from $\partial\Omega$. At weak coupling, the covectors normal to these surfaces will be timelike w.r.t. $\hat{g}^{\mu\nu}$ and $\tilde{g}^{\mu\nu}$ (since this is the case in GR), which implies that these physical characteristic surfaces are spacelike (i.e. "superluminal") w.r.t. $\hat{g}^{\mu\nu}$ and $\tilde{g}^{\mu\nu}$. Thus the Cauchy horizon of Ω will be one of these physical characteristic surfaces rather than one of the unphysical characteristic surfaces that is null w.r.t. $\hat{g}^{\mu\nu}$ or $\tilde{g}^{\mu\nu}$.

We expect that, generically, this innermost ingoing physical characteristic surface will be spacelike also w.r.t. $g^{\mu\nu}$ (as for the examples in [59]). Thus generically we expect the Cauchy horizon of Ω to be spacelike w.r.t. the physical metric $g^{\mu\nu}$. It would be

[8]See Ref. [95] for results supporting this expectation for the case of a quasilinear strongly hyperbolic system.

interesting to study properties of this Cauchy horizon and the domain of dependence $\mathcal{D}(\Omega)$ in more detail.

Appendix 3.A Maxwell theory in modified Lorenz gauge

In this section we will discuss the analogue of our new formulation of GR in the simpler setting of Maxwell theory. The presentation follows closely our discussion of modified harmonic gauge GR in section 3.2.

3.A.1 Equation of motion

The vacuum Maxwell equations for the (antisymmetric) electromagnetic field tensor $F^{\mu\nu}$ on a globally hyperbolic (d dimensional) spacetime (M, g) are

$$E^\mu = 0 \tag{3.113}$$

with

$$E^\mu \equiv \nabla_\nu F^{\mu\nu} \tag{3.114}$$

and the Bianchi identity for F

$$\nabla_{[\rho} F_{\mu\nu]} = 0 \tag{3.115}$$

which implies that $F_{\mu\nu}$ can be written (locally) as the exterior derivative of a potential 1-form A:

$$F_{\mu\nu} = \nabla_\mu A_\nu - \nabla_\nu A_\mu. \tag{3.116}$$

Let $\tilde{g}^{\mu\nu}$ be an (inverse) Lorentzian metric on M and let

$$H \equiv -\tilde{g}^{\alpha\beta} \nabla_\beta A_\alpha \tag{3.117}$$

Our modified Lorenz gauge condition is then

$$H = 0. \tag{3.118}$$

We introduce another (inverse) Lorentzian metric $\hat{g}^{\mu\nu}$ to write the gauge-fixed Maxwell equations as

$$E^\mu_{\mathrm{mLg}} = 0 \tag{3.119}$$

where $E^\mu_{\rm mLg}$ is defined by

$$E^\mu_{\rm mLg} = E^\mu + \hat{g}^{\mu\nu}\nabla_\nu H. \tag{3.120}$$

Now the gauge-fixed equations for A_μ can be written as

$$E^\mu_{\rm mLg} \equiv -g^{\mu\nu}g^{\rho\sigma}\nabla_\rho\nabla_\sigma A_\nu + g^{\mu\rho}\nabla_\rho\left(g^{\nu\sigma}\nabla_\sigma A_\nu\right) - \hat{g}^{\mu\rho}\nabla_\rho\left(\tilde{g}^{\nu\sigma}\nabla_\sigma A_\nu\right) = 0 \tag{3.121}$$

In conventional Lorenz gauge $g^{\mu\nu} = \hat{g}^{\mu\nu} = \tilde{g}^{\mu\nu}$ and the second and third term in the above equation cancel, leaving a simple wave equation for A. We assume that the null cones of the three metrics are related as in Fig. 3.1.

3.A.2 Propagation of the gauge condition

To show that the gauge condition (3.118) is propagated we follow a standard argument similar to the original Lorenz gauge case (and analogous to the harmonic gauge GR case). We assume that we have a solution of (3.119) on M and consider the identity

$$\nabla_\mu E^\mu = \nabla_\mu\nabla_\nu F^{\mu\nu} = 0 \tag{3.122}$$

that is a consequence of the antisymmetry of $F^{\mu\nu}$. Using this we have

$$0 = \nabla_\mu E^\mu_{\rm mLg} = \hat{g}^{\mu\nu}\nabla_\mu\nabla_\nu H + \left(\nabla_\mu\hat{g}^{\mu\nu}\right)\nabla_\nu H \tag{3.123}$$

which is a homogeneous linear wave equation for H.

Given initial data specified on a surface Σ spacelike w.r.t. $g^{\mu\nu}$ and hence also w.r.t. $\hat{g}^{\mu\nu}$ and $\tilde{g}^{\mu\nu}$, one can impose the gauge condition $H = 0$ initially and then the constraint equation $n_\mu E^\mu = 0$ (where n_μ is normal to the hypersurface) implies that $n \cdot \partial H = 0$ initially. Hence, by well-posedness of (3.123), H vanishes throughout $\hat{D}(\Sigma)$ and therefore also throughout $D(\Sigma) \subset \hat{D}(\Sigma)$. So any solution of (3.119) arising from initial data satisfying the constraint equation and the gauge condition will also satisfy $E^\mu = 0$ in $D(\Sigma)$.

3.A.3 Strong hyperbolicity

The principal symbol of (3.119) acting on a covector t_μ is given by

$$\mathcal{P}(\xi)^{\mu\nu}t_\nu = \mathcal{P}_\star(\xi)^{\mu\nu}t_\nu + \mathcal{P}_{\rm GF}(\xi)^{\mu\nu}t_\nu \tag{3.124}$$

with

$$\mathcal{P}_\star(\xi)^{\mu\nu}t_\nu = -g^{\mu\nu}g^{\gamma\delta}\xi_\gamma\xi_\delta t_\nu + g^{\mu\gamma}g^{\nu\delta}\xi_\gamma\xi_\delta t_\nu \tag{3.125}$$

and

$$\mathcal{P}_{\mathrm{GF}}(\xi)^{\mu\nu}t_\nu = -\hat{g}^{\mu\gamma}\tilde{g}^{\nu\delta}\xi_\gamma\xi_\delta t_\nu \tag{3.126}$$

As for GR, our task is to show that $M(\xi_i)$ has real eigenvalues and possesses a complete set of eigenvectors with smooth dependence on the unit vector ξ_i. This boils down to studying the characteristic equation

$$P(\xi)^{\mu\nu}t_\nu = 0. \tag{3.127}$$

In analogy with the GR case, for any ξ_μ, we have

$$\xi_\mu\mathcal{P}_\star(\xi)^{\mu\nu} = 0. \tag{3.128}$$

Therefore, by considering

$$0 = \xi_\mu\mathcal{P}(\xi)^{\mu\nu}t_\nu = \xi_\mu\mathcal{P}_{\mathrm{GF}}(\xi)^{\mu\nu}t_\nu = (\hat{g}^{\mu\gamma}\xi_\mu\xi_\gamma)\left(\tilde{g}^{\nu\delta}\xi_\delta t_\nu\right) \tag{3.129}$$

we find that at least one of the following two cases must hold: (i) $\tilde{g}^{\nu\delta}\xi_\delta t_\nu = 0$ or (ii) $\hat{g}^{\mu\gamma}\xi_\mu\xi_\gamma = 0$.

The physical interpretation of case (i) is a high-frequency wave with polarization t_μ and wave vector ξ_μ that satisfies the modified Lorenz gauge condition. Case (i) can be split into two subcases: characteristics falling into this category must have either (ia) $g^{\mu\nu}\xi_\mu\xi_\nu \neq 0$ or (ib) $g^{\mu\nu}\xi_\mu\xi_\nu = 0$. An argument very similar to the one presented in the GR case reveals that characteristics in subcase (ia) satisfy $\tilde{g}^{\mu\nu}\xi_\mu\xi_\nu = 0$ which has two real solutions for ξ_0 depending smoothly on ξ_i. Adopting the notation used in section 3.2.3, we shall denote these solutions by $\tilde{\xi}_0^\pm$. The corresponding polarizations are $t_\mu^\pm = \xi_\mu^\pm \equiv (\tilde{\xi}_0^\pm, \xi_i)$; these are "pure gauge" vectors associated to the residual gauge freedom in (3.118). On the other hand, the modes of subcase (ib) have eigenvalues $\xi_0^\pm$ (obtained by solving $g^{\mu\nu}\xi_\mu\xi_\nu = 0$ for ξ_0). The only requirement on the corresponding eigenvectors is that they be orthogonal to $\xi_\mu^\pm = (\xi_0^\pm, \xi_i)$ in both $\tilde{g}^{\mu\nu}$ and $g^{\mu\nu}$. Hence there are $d-2$ linearly independent eigenvectors in this subclass (for each sign choice in $\xi_0^\pm$). These can be interpreted as the physical photon polarizations. Finally, case (ii) contains the "gauge condition violating" modes whose characteristic covectors denoted by $\hat{\xi}_\mu^\pm = (\hat{\xi}_\mu^\pm, \xi_i)$ are null w.r.t. $\hat{g}^{\mu\nu}$. For each of these covectors there is only one corresponding eigenvector that can be found by following a similar strategy as in the

GR case. In summary, we find that $M(\xi_i)$ has $2d$ real eigenvalues and a complete set of smooth and real eigenvectors which guarantees that (3.119) is strongly hyperbolic.

Strong hyperbolicity of our modified harmonic gauge formulation of GR is robust against deformation of the theory into a weakly coupled Lovelock or Horndeski theory. Similary, strong hyperbolicity of the above formulation of Maxwell theory should be robust against the inclusion of small nonlinear terms, i.e., a weakly coupled theory of nonlinear electromagnetism (with second order equations of motion). The initial value problem for such theories has been studied by writing the equations of motion as a first order system for the field strength tensor $F_{\mu\nu}$. This system is *symmetric* hyperbolic under certain conditions [96]. Our modified Lorenz gauge would provide an alternative well-posed formulation of such theories, with equations written in terms of the potential A_μ instead of the field strength.

Chapter 4

On the construction of asymptotically flat initial data in scalar-tensor effective field theory

The contents of this chapter are based on original research [97] submitted to Physical Review D.

4.1 Introduction

To explore the dynamics of effective theories of gravity that modify GR, it is important to consider another requirement related to the Cauchy problem: the possibility to construct initial data that gives a good approximation of a realistic astrophysical system when evolved in time. Similarly to the initial value problem, this is a mathematical consistency problem that is also relevant for numerical simulations. In this chapter, we investigate this problem in 4∂ST theories (1.5).

In general relativity, the initial data is subject to constraint equations obtained as follows. Let Σ be a spacelike hypersurface in a globally hyperbolic spacetime with (future-directed) unit normal n^μ and let γ be the induced metric on Σ. Then the projections

$$\mathcal{H}^{\rm GR} \equiv G_{\mu\nu}n^\mu n^\nu = 0 \qquad \text{and} \qquad \mathcal{M}^{\rm GR}_\mu \equiv G_{\alpha\beta}n^\alpha\gamma^\beta_\mu = 0 \tag{4.1}$$

of Einstein's equations, called the Hamiltonian and momentum constraints, contain no second time derivatives of the metric. Similarly, in a 4∂ST theory (or more generally, in a Horndeski or Lovelock theory), the projections

$$\mathcal{H} \equiv E_{\mu\nu}n^{\mu}n^{\nu} = 0 \qquad \text{and} \qquad \mathcal{M}_{\mu} \equiv E_{\alpha\beta}n^{\alpha}\gamma^{\beta}_{\mu} = 0 \tag{4.2}$$

of the gravitational equation of motion (1.6) are constraint equations: they contain no second time derivatives of the metric and the scalar field.

It should be noted that it is possible to perform numerical simulations in a 4∂ST theory without a detailed knowledge of the properties of the 4∂ST constraint equations. The dynamics of binary black hole systems in a shift symmetric 4∂ST theory was studied numerically in a recent work of East and Ripley [70]. They focused on the theory with $V(\phi) = f_1(\phi) = 0$ and $f_2(\phi) = \lambda\phi$ (λ is a constant) which admits black hole solutions with scalar hair. The initial data used in [70] is based on the observation that the 4∂ST constraint equations (4.2) reduce to the Hamiltonian and momentum constraints of vacuum general relativity provided that one chooses the initial values of the scalar field and its time derivative to be zero on the entire initial data surface. Hence one can use a general relativistic initial data for a binary black hole system (with a trivial initial scalar field configuration) and evolve this data in time. With the choice of couplings mentioned above, the black holes scalarize dynamically during the evolution. Nevertheless, one may be interested in a more general class of solutions to the constraint equations. For example, one may wish to construct initial data that is closer to a binary system of scalarized black holes.

In general relativity there is a vast literature on the initial data problem (see e.g. [84, 90, 98, 99] and references therein). Most of the successful approaches, such as the conformal transverse traceless (CTT) [100] or the conformal thin sandwich (CTS) [101] method, are based on a conformal rescaling of certain variables. The main idea is that the constraint equations form a system of elliptic partial differential equations (PDEs) in some of these conformally rescaled variables, whereas other variables play the role of freely specifiable sources ("free data"). Once a useful set of variables is identified, the construction of initial data comes down to the following two steps. Firstly, it must be demonstrated that under the right conditions (on the free data and the topology of the initial slice) the elliptic equations yield a unique solution for the rest of the variables.[1]

[1]The failure of uniqueness is not necessarily a problem from a mathematical point of view, as long as one can make a clear interpretation of what each solution represents. However, it might cause

Secondly, the free data must be chosen such that it corresponds to an astrophysically realistic system.

In this chapter, we address these two problems in the context of weakly coupled 4∂ST theories. We apply the above mentioned two conformal methods to 4∂ST gravity and rewrite the 4∂ST constraints in terms of the conformally rescaled variables. Since we are mainly interested in isolated systems such as a binary black hole system, in this chapter we shall study these elliptic equations on asymptotically Euclidean initial slices. Although a general 4∂ST theory does not have as good conformal properties as GR, the implicit function theorem (in Banach spaces) guarantees existence and uniqueness of solutions to the conformally formulated 4∂ST constraints at weak coupling.

A special solution of the conformally formulated constraints of vacuum general relativity is the Bowen-York initial data [103] (and its variations [104]) that is often used in numerical relativity studies to construct approximate initial data for multiple boosted and rotating black holes. The significance of the Bowen-York method is that it provides a simple analytical solution to the momentum constraint and reduces the problem to the numerical integration of the Hamiltonian constraint. We show that the Bowen-York method can be generalized to 4∂ST theories. In this case, we find that the momentum constraint can be solved exactly for the canonical momenta conjugate to the scalar field ϕ and the spatial metric γ_{ij}. This trick reduces the problem of solving the constraints to solving the Hamiltonian constraint and a system of algebraic equations. The role of the extra algebraic equations is to obtain the extrinsic curvature $K_{ij} = -\frac{1}{2}\mathcal{L}_n\gamma_{ij}$ and the quantity $K_\phi = -\frac{1}{2}\mathcal{L}_n\phi$ from the canonical momenta. Once again, the implicit function theorem implies that the resulting system of equation can be solved, at least for small couplings. In numerical relativity applications, this system can be solved iteratively in the couplings.

The chapter is organised as follows. In Section 4.2, we describe the conformal transverse traceless method and extend it to 4∂ST theories. In more detail, section 4.2.1 contains the definition of the conformal variables used throughout this paper and the derivation of the CTT version of the constraint equations in general relativity. Next, in section 4.2.2, we review some mathematical definitions and theorems on the well-posedness of the boundary value problem of the CTT system for asymptotically Euclidean initial data slices. Section 4.2.3 reviews the Bowen-York initial data for general relativity which is based on the CTT constraint equations. The rest of Section 4.2 details the

problems (failure of convergence) in numerical simulations (see e.g. the Summary and discussion section of [102]).

extension of the CTT method to 4∂ST theories. After providing the CTT constraint equations for the scalar-tensor theory (1.5) in section 4.2.4, we state and prove a theorem on the well-posedness of the corresponding boundary value problem. Finally, we conclude the discussion of the CTT approach by presenting an extension of the Bowen-York "puncture" data to 4∂ST theories.

Section 4.3 is concerned with the original conformal thin sandwich method. From a mathematical point of view, this is very similar to the CTT approach. However, the CTS method deserves a separate treatment due to its physical significance. After reviewing the CTS equations that gives the basis of a popular way of initial data construction, we state the corresponding existence and uniqueness theorems on asymptotically Euclidean manifolds both in general relativity and in 4∂ST theories. The section is concluded with some remarks on numerical relativity applications.

Sometimes, an extension of the original conformal thin sandwich method (dubbed as XCTS) is used to find initial data in numerical studies [105]. The significance of this method is that in general relativity it provides an elegant way to construct initial data for a binary black hole spacetime in a corotating coordinate system such that the black holes move along quasicircular orbits. However, the mathematical theory of the extended CTS system is more complicated than in the case of the CTT or the original CTS methods. In particular, it is known that this system fails to have a unique solution for certain choices of the "free data". For this reason, we merely put forward a proposal on how to adapt the extended CTS approach to 4∂ST theories and we only briefly discuss the expected properties of the resulting system.

Appendices 4.A and 4.B contain some identities that may be helpful for performing the $3+1$ and conformal decompositions of the 4∂ST equations.

4.2 The conformal transverse traceless decomposition

4.2.1 Description of the method in general relativity

In this section, we review the conformal transverse traceless (CTT) approach introduced by York [100] to construct an asymptotically flat initial data set. Let (M, g) be a smooth, 4-dimensional, globally hyperbolic spacetime. An initial data set is a triple $(\Sigma, \gamma_{ij}, K_{ij})$ where Σ is a smooth 3-dimensional spacelike submanifold of M, γ_{ij} is a Riemannian metric on Σ and K_{ij} is the extrinsic curvature. If n^μ denotes the (future-directed) unit normal to Σ then the extrinsic curvature is defined as

$$K_{ij} = -\frac{1}{2}\mathcal{L}_n\gamma_{ij} \tag{4.3}$$

We say that the initial data set is asymptotically flat if it satisfies the following three requirements. First of all, there exists a compact subset S of Σ such that $\Sigma\backslash S$ is the disjoint union of a finite number of open sets called ends, each of which is diffeomorphic to the complement of a closed ball in $\mathbb{R}^3$. Secondly, in a suitable coordinate system $\gamma_{ij} - \delta_{ij}$ and K_{ij} approach zero at a suitable rate (made more precise in the next subsection) as $r \equiv \sqrt{x^i x^i} \to \infty$. Furthermore, we require that the initial data set satisfies the constraint equations of the Einstein-matter equation (with the convention $16\pi G = 1$)

$$G_{\mu\nu} = \frac{1}{2}T_{\mu\nu} \tag{4.4}$$

with some energy-momentum tensor $T_{\mu\nu}$: the Hamiltonian constraint

$$\mathcal{H} \equiv \frac{1}{2}\left(R[D] + \gamma^{i_1 i_2}_{j_1 j_2} K_{i_1}{}^{j_1} K_{i_2}{}^{j_2} - \varrho\right) = 0 \tag{4.5}$$

and the momentum constraint

$$\mathcal{M}^i \equiv \gamma^{ii_1}_{jj_1} D^j K_{i_1}{}^{j_1} - \frac{1}{2}\mathfrak{p}^i = 0. \tag{4.6}$$

In these equations, D is the covariant derivative associated with γ, $R[D]$ is the corresponding Ricci scalar, ϱ and $\mathfrak{p}^i$ are the energy and momentum densities of $T_{\mu\nu}$, i.e.

$$\varrho \equiv T_{\mu\nu}n^\mu n^\nu, \qquad \mathfrak{p}^i \equiv T_{\mu\nu}n^\mu\gamma^{i\nu}, \tag{4.7}$$

and finally,

$$\gamma^{i_1\ldots i_n}_{j_1\ldots j_n} \equiv n!\gamma^{i_1}_{[j_1}\ldots\gamma^{i_n}_{j_n]} \tag{4.8}$$

To construct an initial data set obeying the above conditions, we follow the recipe of York and perform a conformal transformation on the metric γ, with conformal factor ψ. The conformal metric will be denoted by $\tilde{\gamma}$:

$$\gamma_{ij} = \psi^4\tilde{\gamma}_{ij}. \tag{4.9}$$

The inverse of $\tilde{\gamma}_{ij}$ will be denoted by $\tilde{\gamma}^{ij}$ so that $\tilde{\gamma}^{ij} = \psi^4\gamma^{ij}$. In particular, note that $\tilde{\gamma}^{ij} \neq \tilde{\gamma}_{kl}\gamma^{ik}\gamma^{jl}$! Henceforth, indices of tensor fields whose notations contain a tilde will be raised and lowered with $\tilde{\gamma}^{ij}$ and $\tilde{\gamma}_{ij}$, respectively. On the other hand, indices of tensor fields denoted by letters without a tilde will be raised and lowered using γ.

It is useful to decompose K_{ij} to a trace part and a traceless part as

$$K_{ij} = \psi^{-2}\tilde{A}_{ij} + \frac{1}{3}K\gamma_{ij} \tag{4.10}$$

with $K \equiv \gamma^{ij}K_{ij}$. Using the new variables $(\psi, \tilde{\gamma}, \tilde{A}, K)$, the Hamiltonian constraint can be rewritten as

$$-\frac{1}{4}\psi^5\mathcal{H} \equiv \tilde{\gamma}^{kl}\tilde{D}_k\tilde{D}_l\psi - \frac{1}{8}\psi R[\tilde{D}] - \frac{1}{12}\psi^5K^2 + \frac{1}{8}\psi^{-7}\tilde{A}_{kl}\tilde{A}^{kl} + \frac{1}{8}\psi^{-3}\tilde{\varrho} = 0 \tag{4.11}$$

This conformal version of the Hamiltonian constraint is called the Lichnerowicz equation. One can also rewrite the momentum constraint using the new variables as

$$\psi^{10}\mathcal{M}^i \equiv \tilde{D}_j\tilde{A}^{ij} - \frac{2}{3}\psi^6\tilde{\gamma}^{ij}\tilde{D}_jK - \frac{1}{2}\tilde{p}^i = 0. \tag{4.12}$$

Here, $\tilde{D}$ is the covariant derivative associated with $\tilde{\gamma}$, $R[\tilde{D}]$ is the corresponding Ricci scalar and we additionally introduced the conformally rescaled energy and momentum density

$$\tilde{\varrho} \equiv \psi^8\varrho \qquad\qquad \tilde{\mathfrak{p}}^i \equiv \psi^{10}\mathfrak{p}^i. \tag{4.13}$$

There are two main reasons for choosing this particular scaling. The first one is a mathematical reason: this scaling is well-suited for proofs of existence and uniqueness of the constraint system. Secondly, it has some physical significance as well: if $(\tilde{\varrho}, \tilde{\mathfrak{p}}^i)$ satisfies the dominant energy condition

$$\tilde{\varrho} \geq \sqrt{\tilde{\gamma}_{ij}\tilde{\mathfrak{p}}^i\tilde{\mathfrak{p}}^j}$$

then so does the physical energy and momentum densities, i.e.

$$\varrho \geq \sqrt{\gamma_{ij}\mathfrak{p}^i\mathfrak{p}^j}$$

If the matter source is a real scalar field then it is useful to define

$$K_\phi \equiv -\frac{1}{2}\mathcal{L}_n\phi, \qquad\qquad \tilde{K}_\phi \equiv \psi^6K_\phi \tag{4.14}$$

in analogy with the extrinsic curvature. For a minimally coupled scalar field (theory (1.5) with $\epsilon_1, \epsilon_2 = 0$), one can express the energy and momentum densities of the scalar field in terms of the conformal variables

$$\varrho = \frac{1}{2}\left(4\psi^{-12}\tilde{K}_\phi^2 + \psi^{-4}\tilde{\gamma}^{ij}\partial_i\phi\partial_j\phi\right) + V(\phi) \quad (4.15)$$

$$\mathfrak{p}^i = 2\psi^{-10}\tilde{K}_\phi\tilde{\gamma}^{ij}\partial_i\phi \quad (4.16)$$

We can see that in the expression for ϱ there are terms with different conformal scaling and hence for a scalar field it is not necessarily beneficial to use the variable $\tilde{\varrho}$ of equation (4.13). However, $\mathfrak{p}^i$ is York-scaled with

$$\tilde{\mathfrak{p}}^i = 2\tilde{K}_\phi\tilde{\gamma}^{ij}\partial_i\phi. \quad (4.17)$$

To solve the momentum constraint, York proposed a decomposition of the conformal extrinsic curvature $\tilde{A}_{ij}$ to a longitudinal and transverse-traceless (TT) part

$$\tilde{A}^{ij} = \tilde{A}^{ij}_{\mathrm{TT}} + \tilde{A}^{ij}_{\mathrm{L}} \quad (4.18)$$

To make it clear, the tracelessness and the transversality of $\tilde{A}_{\mathrm{TT}}$ can be expressed as

$$\tilde{\gamma}_{ij}\tilde{A}^{ij}_{\mathrm{TT}} = 0 \qquad \tilde{D}_i\tilde{A}^{ij}_{\mathrm{TT}} = 0 \quad (4.19)$$

As explained below, the longitudinal piece $\tilde{A}_L$ can be expressed as the action of the *conformal Killing operator* $\tilde{L}$ on a vector field Y^i, that is,

$$\tilde{A}^{ij}_L = (\tilde{L}Y)^{ij} \equiv \tilde{D}^iY^j + \tilde{D}^jY^i - \frac{2}{3}\tilde{\gamma}^{ij}\tilde{D}_kY^k \quad (4.20)$$

The existence and uniqueness of such a decomposition hinges on the existence and uniqueness of the solution to the equation

$$\tilde{\Delta}_LY^i = \tilde{D}_j\tilde{A}^{ij} \quad (4.21)$$

where the differential operator $\tilde{\Delta}_L$ is called the *conformal vector Laplacian* and it can be defined with its action on a vector field

$$\tilde{\Delta}_LY^i \equiv \tilde{D}_j(\tilde{L}Y)^{ij} = \tilde{D}_j\tilde{D}^jY^i + \frac{1}{3}\tilde{D}^i\tilde{D}_jY^j + \tilde{R}^i{}_jY^j. \quad (4.22)$$

In terms of the variables $(Y, \tilde{\gamma}, \tilde{K})$, the momentum constraint is

$$\tilde{\Delta}_LY^i - \frac{2}{3}\psi^6\tilde{\gamma}^{ij}\tilde{D}_jK = \frac{1}{2}\tilde{\mathfrak{p}}^i \quad (4.23)$$

We can see that the advantage of the variables $(\psi, \tilde{\gamma}, \tilde{A}_{\text{TT}}, K, Y)$ is that the Hamiltonian and the momentum constraints take the form of a system of four elliptic partial differential equations consisting of (4.11) and (4.23). These equations are to be solved for the variables (ψ, Y). The rest of the variables $(\tilde{\gamma}, \tilde{A}_{\text{TT}}, K)$ play the role of sources to be chosen freely.

In general relativity, it has been demonstrated [90] that the above procedure actually leads to a unique asymptotically flat initial data set for a suitable choice of $(\tilde{\gamma}, \tilde{A}_{\text{TT}}, K)$. In the next subsection, we review some theorems (for both vacuum gravity and gravity minimally coupled to a scalar field) containing conditions on the free data that guarantee the existence of a unique solution for (ψ, Y) with the desired regularity and asymptotic fall-off.

4.2.2 Mathematical results in general relativity

We continue the discussion by stating some of the previous statements in a mathematically more precise form (see e.g. [90] and references therein). We begin with a brief discussion of weighted Sobolev spaces that capture the desired asymptotic fall-off requirements. In this section, we consider initial data surfaces of $n \geq 3$ dimensions.

Given coordinates x^i on the initial slice Σ, let $\sigma(x) \equiv (1 + |x|^2)^{1/2}$ with $|x| \equiv \sqrt{\delta_{ij} x^i x^j}$ and let $1 \leq p \leq \infty$, $\delta \in \mathbb{R}$, $s \in \mathbb{N}$. Given a tensor field u of some given type on Σ, one may define the weighted Sobolev norm

$$||u||_{p,s,\delta} \equiv \sum_{0 \leq |m| \leq s} ||\sigma^{|m|+\delta}(x) D^m u||_{L^p(\Sigma)}. \tag{4.24}$$

Then we say that the weighted Sobolev space $W^p_{s,\delta}(\Sigma)$ is the space of tensor fields on Σ whose norm $|| \cdot ||_{p,s,\delta}$ is finite. If Σ is a 3-manifold and a tensor field u on Σ is in $W^p_{s,\delta}(\Sigma)$, then it must fall off faster than $r^{-\delta-3/p}$ as $r \to \infty$ and similarly its derivatives $D^m u$ must fall off faster than $r^{-\delta-3/p-|m|}$. Hence, the role of the parameter δ is to provide additional information on the the asymptotic behaviour of the tensor field.

Now we can define the notion of an asymptotically Euclidean manifold endowed with a Riemannian metric in a certain weighted Sobolev class.

Definition 4.1. An n-dimensional manifold (M, γ) is said to be *asymptotically Euclidean of class* $W^p_{\sigma,\rho}$ if

(i) There exists a finite number of open sets $\{E_I\}$ called ends, a compact set S and a set of diffeomorphisms $\{\Phi_I\}$ such that $\Sigma \backslash S = \bigcup_I E_I$ and Φ_I maps each E_I to a complement of a closed ball in $\mathbb{R}^n$.

(ii) In each end $(\Phi_I^\star \gamma)_{ij} - \delta_{ij} \in W^p_{\sigma,\rho}$ with $\sigma > \frac{n}{p}$ and $\rho > -n/p$.

Requirement (ii) in the above definition captures the condition that (in asymptotically Euclidean coordinate system) the components of the metric are $\gamma_{ij} = \delta_{ij} + \mathcal{O}(r^{-\lambda})$ as $r \to \infty$ where λ is an arbitrary positive real number. This is a less restrictive condition than the usual assumption of $\gamma_{ij} = \delta_{ij} + \mathcal{O}(r^{-1})$. In the following lemma we collect some of the useful properties of weighted Sobolev spaces [106, 107].

Lemma 4.1. *Properties of weighted Sobolev spaces.*

(i) Let $s > \frac{n}{p} + k$. Then $W^p_{s,\delta}(\mathbb{R}^n) \subset C^k(\mathbb{R}^n)$.

(ii) Pointwise multiplication satisfies $W^p_{s_1,\delta_1}(\Sigma) \times W^p_{s_2,\delta_2}(\Sigma) \to W^p_{s_3,\delta_3}(\Sigma)$ provided that $s_3 < s_1 + s_2 - \frac{n}{p}$ and $\delta_3 < \delta_1 + \delta_2 + \frac{n}{p}$.

Moreover, let $p > 1$, $s > \frac{n}{p}$, $0 \leq l \leq s$ and define

$$W^p_{s,\delta}(1, \Sigma) = \left\{ f : \Sigma \to \mathbb{R} \ : \ f - 1 \in W^p_{s,\delta}(\Sigma) \right\}. \tag{4.25}$$

Then pointwise multiplication induces smooth maps

$$W^p_{s,\delta}(1, \Sigma) \times W^p_{s-l,\delta+l}(\Sigma) \to W^p_{s-l,\delta+l}(\Sigma) \tag{4.26}$$

$$W^p_{s,\delta}(1, \Sigma) \times W^p_{s-l,\delta+l}(1, \Sigma) \to W^p_{s-l,\delta+l}(1, \Sigma) \tag{4.27}$$

Part (i) of this lemma just tells us that a sufficiently weighted Sobolev-regular tensor field are (k times) continuously differentiable. The rough version of the second part of the lemma implies the following. Given a tensor field T which is expressed as a contraction (pointwise multiplication) of several sufficiently regular tensor fields S_A (i.e. $S_A \in W^p_{s_A,\delta_A}(\Sigma)$ and s_A is large enough). Then the weighted Sobolev regularity of T is the same as that of the least regular factor S_A.

Now let us turn to the actual discussion of the conformally formulated constraint equations and state some previous results. We start with the momentum constraint.

Theorem 4.1. *Let (Σ, γ) be a $W^p_{s,\delta}$ asymptotically Euclidean manifold with $p > \frac{n}{2}$, $s > \frac{n}{p}$ and $-\frac{n}{p} < \delta < n - 2 - \frac{n}{p}$. Assume that we are given $\tilde{A}_{\mathrm{TT}} \in W^p_{s-1,\delta+1}(\Sigma)$.*

(i) Consider the case of maximal slicing $K \equiv 0$. *Then the constraints decouple and the momentum constraint has a unique solution* $Y \in W^p_{s,\delta}(\Sigma)$.

(ii) Consider the case of nonzero $K \in W^p_{s-1,\delta+1}(\Sigma)$ *and suppose that we are given* $\psi > 0$, $\psi \in W^p_{s,\delta}(1,\Sigma)$. *Then the momentum constraint has a unique solution* $Y \in W^p_{s,\delta}(\Sigma)$.

Next we turn to the Lichnerowicz equation which is highly nonlinear and therefore more subtle. We specifically concentrate on the vacuum case and assume that Σ is a maximal slice. Similar results hold when Σ has (nearly or exactly) constant mean curvature. Before stating the theorem on the Lichnerowicz equation, we need to discuss a topological condition on the initial data surface to ensure uniqueness.

Consider an n-dimensional asymptotically Euclidean manifold (Σ, γ) of class $W^p_{s,\delta}(\Sigma)$. We say that such a manifold is in the *positive Yamabe class* if the functional

$$I_\gamma[f] \equiv \int_\Sigma d^n x \sqrt{\gamma} \left[\gamma^{ij}\partial_i f \partial_j f + \frac{1}{8} R[\tilde{D}] f^2\right] > 0 \tag{4.28}$$

is positive for every nontrivial function f of type $W^p_{2,\rho}(\Sigma)$ with $\rho > -\frac{n}{p} + \frac{n}{2} - 1$. Interestingly, the functional $I_\gamma[f]$ is conformally invariant in the sense that

$$I_\gamma[f] = I_{\gamma'}[f'], \qquad \gamma' = \theta^{\frac{4}{n-2}}\gamma, \qquad f' = \theta^{-1} f \tag{4.29}$$

Theorem 4.2. *We make the following hypotheses.*

(i) Let $(\Sigma, \tilde{\gamma})$ *be an* n*-dimensional asymptotically Euclidean manifold of type* $W^p_{s,\delta}$ *with*

$$p > \frac{n}{2}, \qquad s > \frac{n}{p} \qquad \text{and} \qquad -1 + \frac{n}{2} - \frac{n}{p} < \delta < -2 + n - \frac{n}{p}.$$

(ii) Assume that we are given $\tilde{A}_{TT} \in W^p_{s-1,\delta+1}(\Sigma)$ *and* $K = 0$ *as free data.*

(iii) Suppose that $(\Sigma, \tilde{\gamma})$ *is in the positive Yamabe class.*

(iv) Finally, assume that we are given a vector field $Y \in W^p_{s,\delta}(\Sigma)$.

Under hypotheses (i)-(iv) the Lichnerowicz equation has a unique solution $\psi > 0$ *with* $\psi \in W^p_{s,\delta}(1,\Sigma)$.

Note that there are different versions of the above theorem which do not require the data to be of the positive Yamabe class but in those cases the other conditions are more restrictive (see [90] for a more complete account).

Consider now the case when we include a minimally coupled scalar field with nonnegative potential $V(\phi) \geq 0$. As noted in (4.15), ϱ contains terms with different conformal scalings, introducing "bad" terms in the Lichnerowicz equation. Nevertheless, one still has the following theorem [108].

Theorem 4.3. *Let* (Σ, γ) *be a* 3*-dimensional asymptotically Euclidean manifold of class* $W^p_{s,\delta}$ *with* $K = 0$*,* $s > 2 + \frac{3}{p}$ *and* $\delta > -\frac{3}{p}$*. We further require that*

$$R[\tilde{D}] - \frac{1}{2}\tilde{\gamma}^{ij}\partial_i\phi\partial_j\phi > 0.$$

Then there exists an open set of values for the free data $(\tilde{A}_{TT}, \phi, \tilde{K}_\phi)$ *satisfying* $\phi - \phi_\infty \in W^p_{s,\delta}(\Sigma)$ *where* ϕ_∞ *is the asymptotic (constant) value of the scalar field,* $\tilde{A}_{TT}, \tilde{K}_\phi \in W^p_{s-1,\delta+1}(\Sigma)$ *and* $V(\phi) \in W^p_{s-2,\delta+2}(\Sigma)$ *such that the Lichnerowicz equation has a solution* $\psi > 0$ *of class* $W^p_{s,\delta}(1, \Sigma)$*.*

It is worth pointing out that even though Theorem 4.3 allows for ϕ to have a non-zero asymptotic value, the requirement $V(\phi) \in W^p_{s-2,\delta+2}(\Sigma)$ implies that we must have $V(\phi_\infty) = 0$. Of course, in general, $\phi \in W^p_{s,\delta}$ does not imply $V(\phi) \in W^p_{s-2,\delta+2}$. In fact, this condition puts an implicit constraint on V. However, it also shows that V does not need to be a smooth function.

Finally, we state the corresponding results for the full CTT system of constraints. In the vacuum case, assuming $K = 0$, the Hamiltonian and momentum constraints decouple so combining theorems 4.1 and 4.2 leads to

Theorem 4.4. *Suppose that the hypotheses (i)-(iii) of Theorem 4.2 hold. Then the CTT system of constraint equations (*(4.11) *and* (4.23) *with* $\tilde{\varrho}, \tilde{\mathfrak{p}} = 0$*) admits a unique solution* $\psi \in W^p_{s,\delta}(1, \Sigma)$*,* $Y \in W^p_{s,\delta}(\Sigma)$ *with* $\psi > 0$*.*

Similarly, in the case of gravity minimally coupled to a scalar field, we have

Theorem 4.5. *Let* (Σ, γ) *be a* 3*-dimensional asymptotically Euclidean manifold of class* $W^p_{s,\delta}$ *with* $K = 0$*,* $p > \frac{3}{2}$*,* $s > 2 + \frac{3}{p}$ *and* $1 - \frac{3}{p} > \delta > -\frac{3}{p}$*. Moreover, suppose*

$$R[\tilde{D}] - \frac{1}{2}\tilde{\gamma}^{ij}\partial_i\phi\partial_j\phi > 0.$$

Then there is an open set of values for $(\tilde{A}_{TT}, \phi, \tilde{K}_\phi)$ *satisfying* $\phi - \phi_\infty \in W^p_{s,\delta}(\Sigma)$, $\tilde{A}_{TT}, \tilde{K}_\phi \in W^p_{s-1,\delta+1}(\Sigma)$ *and* $V(\phi) \in W^p_{s-2,\delta+2}(\Sigma)$ *such that the conformally formulated constraints have a solution* (ψ, Y) *with* $\psi \in W^p_{s,\delta}(1, \Sigma)$, $\psi > 0$ *and* $Y \in W^p_{s,\delta}(\Sigma)$.

4.2.3 Bowen-York initial data in general relativity

The theorems presented in the previous section provide the mathematical underpinning of the construction of initial data in general relativity (in vacuum and with a minimally coupled scalar field). It remains to find a suitable choice of free data such that the corresponding solution represents physical systems of interest. A proposal for the choice of free data that yields a slice of a spacetime with multiple black holes (in vacuum) was originally put forward by Bowen and York [103]. Their approach was later modified to better suit for numerical relativity purposes, see e.g. [104]. We briefly review this latter approach.

First of all, let the initial hypersurface Σ be $\mathbb{R}^3$ with a puncture at the origin, i.e. $\Sigma = \mathbb{R}^3 \backslash \{O\}$. Furthermore, consider the simple choice

$$\tilde{\gamma}_{ij} = \delta_{ij}, \qquad K = 0, \qquad \tilde{A}^{ij}_{TT} = 0 \tag{4.30}$$

and assume that we are in vacuum, i.e. $\tilde{\varrho} = 0$, $\tilde{\mathfrak{p}}^i = 0$. Then as shown in [103] one can obtain the following 6-parameter family of analytical solutions to the momentum constraint

$$Y^i = -\frac{1}{4r}\left(7P^i + P^j \hat{x}_j \hat{x}^i\right) - \frac{1}{r^2}\epsilon^{ijk} S_j \hat{x}_k \tag{4.31}$$

where x^i are the usual Euclidean coordinates on $\mathbb{R}^3$, $r = \sqrt{\delta_{ij} x^i x^j}$ is the Euclidean distance from the origin, $\hat{x}^i \equiv x^i / r$ and ϵ^{ijk} is the Levi-Civita tensor associated with the flat metric. The vectors P^i and S^i are to be chosen freely. The corresponding conformal extrinsic curvature is

$$\tilde{A}_{ij}(P,S) = \frac{3}{2r^2}\left(P_i \hat{x}_j + P_j \hat{x}_i - (\gamma_{ij} - \hat{x}_i \hat{x}_j) P^k \hat{x}_k\right) + \frac{3}{r^3}\left(\epsilon_{ikl} S^k \hat{x}^l \hat{x}_j + \epsilon_{jkl} S^k \hat{x}^l \hat{x}_i\right) \tag{4.32}$$

Interestingly, the ADM linear momentum of this data with $S^i = 0$ is

$$P^i_{\mathrm{ADM}} = \frac{1}{8\pi} \int_{S_\infty} \mathrm{d}A \; (K^{ij} - K\gamma^{ij}) \hat{x}_j = P^i, \tag{4.33}$$

and the components of the canonical angular momentum of the solution with $P^i = 0$ are

$$J^i = \frac{1}{8\pi} \int\limits_{S_\infty} \mathrm{d}A \; (K_{jk} - K\gamma_{jk})\epsilon^{ijl} x_l \hat{x}^k = S^i. \tag{4.34}$$

Note that since the momentum constraint is linear in Y and the solution (4.32) is linear in (P, S), a linear superposition of any number of such solutions is also a solution to the momentum constraint. More precisely, if the initial slice is $\mathbb{R}^3$ with N punctures at coordinate locations $c^i_{(\alpha)}$ then

$$\begin{aligned}\tilde{A}^{ij} \;=& \sum_{\alpha=1}^{N} \left[\frac{3}{2r^2_{(\alpha)}}\left(P^i_{(\alpha)}\hat{x}^j_{(\alpha)} + P^j_{(\alpha)}\hat{x}^i_{(\alpha)} - \left(\delta^{ij} - \hat{x}^i_{(\alpha)}\hat{x}^j_{(\alpha)}\right)\right)\right. \\ &\left. + \frac{3}{r^3_{(\alpha)}}\left(\epsilon^i{}_{kl} S^k_{(\alpha)}\hat{x}^l_{(\alpha)}\hat{x}^j_{(\alpha)} + \epsilon^j{}_{kl} S^k_{(\alpha)}\hat{x}^l_{(\alpha)}\hat{x}^i_{(\alpha)}\right)\right]\end{aligned} \tag{4.35}$$

with $r_{(\alpha)} \equiv |x - c_{(\alpha)}|$ and $\hat{x}_{(\alpha)} \equiv \left(x - c_{(\alpha)}\right)/r_{(\alpha)}$ is an exact solution of (4.23) (provided that $K = 0$ and $\tilde{p}^i = 0$). Clearly, in this case $P_{(\alpha)}$ and $S_{(\alpha)}$ represent the ADM linear and angular momenta of the black holes in case of large separation.

Although the momentum constraint has an exact solution, the Hamiltonian constraint is nonlinear and there is no closed formula known for the corresponding solution. However, one can seek the solution in the form

$$\psi = 1 + \frac{1}{\mu} + u, \qquad\qquad \frac{1}{\mu} \equiv \sum_{\alpha=1}^{N} \frac{m_{(\alpha)}}{2|x - c_{(\alpha)}|} \tag{4.36}$$

where the parameters $m_{(\alpha)}$ are called the bare masses of the punctures. The significance of the ansatz (4.36) is that ψ is separated to two pieces: $1/\mu$ is singular at the punctures, whereas u turns out to be regular in the *entire* $\mathbb{R}^3$.

To show that the solution for u is indeed regular, one needs to formulate an elliptic boundary value problem for u on $\mathbb{R}^3$. This amounts to rewriting the Lichnerowicz equation in terms of u and complementing it with a boundary condition at $r \to \infty$. It is worth emphasizing that since this problem is solved for u on $\mathbb{R}^3$ without excising the punctures, no interior boundary conditions are required for u. Since the flat Laplacian annihilates $1 + 1/\mu$ (away from the punctures), the boundary value problem to be solved for u is

$$\Delta u + \frac{1}{8}\mu^7 \tilde{A}_{ij}\tilde{A}^{ij}\Big(1+\mu(1+u)\Big)^{-7} = 0 \tag{4.37}$$

$$\lim_{r\to\infty} \partial_r(ru) = 0 \tag{4.38}$$

where $\tilde{A}^{ij}$ is given by (4.35). The boundary condition for u guarantees that $u = \mathcal{O}(r^{-1})$ as $r \to \infty$ which corresponds to the original notion of asymptotic flatness.

As discussed in [104], this elliptic boundary value problem admits a unique C^2 solution[2] on $\mathbb{R}^3$ (including the punctures). An important part of the proof is to observe that $\mu^7 \tilde{A}_{ij}\tilde{A}^{ij}$ scales as $|x - c_{(\alpha)}|$ and therefore, in the elliptic equation (4.37) the nonlinear term has a continuous prefactor.

The solution represents a compactification of $N+1$ asymptotically flat ends where each puncture corresponds to spatial infinity. Another interesting property of the solution is that in the post-Newtonian (PN) approximation of the two-body point mass system the leading order contribution to the conjugate momentum is exactly of the Bowen-York form, provided that one uses the so-called ADMTT gauge condition [109]. This means that up to third order in the velocities (i.e. of order $(v/c)^3$) the superposition of two Bowen-York extrinsic curvatures represents a slowly moving binary black hole system with large separations. Note however, that this is not true for finite P and J: in particular, a single angular momentum source is not exactly a slice of the Kerr solution, but rather it contains some additional junk radiation. This unphysical gravitational wave content is significant when the separation of the black holes is not large enough or the momenta P, J are not small enough. If one wishes to construct initial data for a binary system with relatively small separation, moving along quasicircular orbits, then the puncture data may not be suitable. One way to improve on the data would be to include higher order PN corrections in the free part of the data [109]. A different approach to construct data that represents a binary system in quasiequilibrium will be presented later. Nevertheless, the puncture approach serves as a fairly good initial data provided that one can afford to simulate a sufficient number of orbits so that there is time for the junk radiation to disperse.

[2]In more detail, the solution is $u \in W^p_{3,\delta}(\mathbb{R}^3)$ with $p > 3$ and $0 \leq \delta < 1 - \frac{3}{p}$. Lemma 4.1 then guarantees that u is C^2.

4.2.4 Conformal transverse traceless decomposition for scalar-tensor EFT

We now turn our attention to the scalar-tensor theory (1.5) and extend previous results (reviewed in sections 4.2.1-4.2.3) to these theories.

We start by giving the constraint equations of the theory (1.5). (These equations can also be found in e.g. [110, 111] for the theory $\epsilon_1 = 0$.) The Hamiltonian constraint can be written as

$$\begin{aligned} 2\mathcal{H} \ \equiv \ & R[D] + \gamma^{i_1 i_2}_{j_1 j_2} K_{i_1}{}^{j_1} K_{i_2}{}^{j_2} - V(\phi) - \frac{1}{2}(D\phi)^2 - 2K_\phi^2 - \epsilon_1 f_1(\phi) X \left(6K_\phi^2 + \frac{1}{2}(D\phi)^2\right) \\ & -2\epsilon_2 \gamma^{i_1 i_2 i_3}_{j_1 j_2 j_3} \left(R[D]_{i_1 i_2}{}^{j_1 j_2} + 2K_{i_1}{}^{j_1} K_{i_2}{}^{j_2}\right) \left(D_{i_3} D^{j_3} f_2(\phi) - 2f_2'(\phi) K_\phi K_{i_3}{}^{j_3}\right) \\ = \ & 0 \end{aligned} \tag{4.39}$$

The momentum constraint has a particularly compact form when written in terms of the canonical momenta:

$$\mathcal{M}_i \equiv D^j \left(\pi_{ij} \gamma^{-1/2}\right) - \frac{1}{2}\pi_\phi \gamma^{-1/2} D_i \phi = 0 \tag{4.40}$$

where the momenta conjugate to ϕ and γ_{ij} are given by

$$\begin{aligned} \frac{\pi_\phi}{\gamma^{1/2}} \ = \ & -2K_\phi(1 + 2\epsilon_1 f_1(\phi) X) \\ & -2\epsilon_2 f_2'(\phi) \gamma^{i_1 i_2 i_3}_{j_1 j_2 j_3} K_{i_1}{}^{j_1} \left(R[D]_{i_2 i_3}{}^{j_2 j_3} + \frac{2}{3} K_{i_2}{}^{j_2} K_{i_3}{}^{j_3}\right) \end{aligned} \tag{4.41}$$

and

$$\begin{aligned} \frac{\pi^i{}_j}{\gamma^{1/2}} \ = \ & \gamma^{i i_1}_{j j_1} K_{i_1}{}^{j_1} + 2\epsilon_2 \gamma^{i i_1 i_2}_{j j_1 j_2} \Big[2K_{i_1}{}^{j_1} D_{i_2} D^{j_2} f_2(\phi) \\ & - f_2'(\phi) K_\phi \left(R[D]_{i_1 i_2}{}^{j_1 j_2} + 2K_{i_1}{}^{j_1} K_{i_2}{}^{j_2}\right)\Big] \end{aligned} \tag{4.42}$$

respectively. After some algebraic manipulations, the momentum constraint can also be written as

$$\begin{aligned} \mathcal{M}^i \ \equiv \ & \gamma^{i i_1}_{j j_1} D^j K_{i_1}{}^{j_1} + K_\phi (1 + 2\epsilon_1 f_1(\phi) X) D^i \phi \\ & + \epsilon_2 \gamma^{i i_1 i_2}_{j j_1 j_2} \Big\{ \left[K_k{}^j D^k f_2(\phi) - 2D^j \left(f_2'(\phi) K_\phi\right)\right] \left(R[D]_{i_1 i_2}{}^{j_1 j_2} + 2K_{i_1}{}^{j_1} K_{i_2}{}^{j_2}\right) \\ & + 4\left(D^j K_{i_1}{}^{j_1}\right) \left(D_{i_2} D^{j_2} f_2(\phi) - 2f_2'(\phi) K_\phi K_{i_2}{}^{j_2}\right) \Big\} = 0 \end{aligned} \tag{4.43}$$

The next step is to follow the recipe of section 4.2.1 and write the constraint equations (4.39)-(4.40) in terms of the variables $(\psi, \tilde{\gamma}_{ij}, K, \tilde{A}^{\mathrm{TT}}_{ij}, Y^i, \phi, \tilde{K}_\phi)$. Clearly, the form of the CTT constraint equations is not quite as elegant as in general relativity: the terms coming from the 4-derivative corrections have different conformal scalings. Nevertheless, the point is that at sufficiently weak couplings, the conformally formulated constraints will constitute a system of elliptic PDEs with a well-posed boundary value problem for the variables (ψ, Y).

By weak couplings, we simply mean that for any (smooth) choice of the functions f_1, f_2, there exists an open set of values for (ϵ_1, ϵ_2) in a neighborhood of $(0, 0)$ such that constraint equations (1.6)-(1.7) yield a solution. In particular, this typically means that the 4-derivative corrections are small compared to the Einstein-minimally coupled scalar terms, or in other words,

$$\epsilon_1 f_1(\phi), \epsilon_1 f_1'(\phi), \epsilon_2 f_2'(\phi), \epsilon_2 f_2''(\phi) \ll \Lambda^2 \tag{4.44}$$

where Λ is any length scale defined by the Riemann tensor and the first and second derivatives of the scalar field.

To discuss the puncture data for 4∂ST theories (later in sections 4.2.6 and 4.2.7), it is useful to conformally rescale the canonical momenta. We introduce

$$\pi_{ij}\gamma^{-1/2} \equiv \psi^{-2}\tilde{\pi}_{ij} + \frac{1}{3}\pi\gamma_{ij}, \qquad \pi_\phi\gamma^{-1/2} \equiv \psi^{-6}\tilde{\pi}_\phi \tag{4.45}$$

The momentum constraint now takes the same form as in general relativity (c.f. (4.12)), after making the substitutions $\tilde{A}_{ij} \to -\tilde{\pi}_{ij}$, $K \to \frac{1}{2}\pi$ and $\tilde{\mathfrak{p}}^i \to -\tilde{\pi}_\phi \tilde{D}^i\phi$:

$$-\tilde{D}_j\tilde{\pi}^{ij} - \frac{1}{3}\psi^6\tilde{\gamma}^{ij}\tilde{D}_j\pi + \frac{1}{2}\tilde{\pi}_\phi\tilde{\gamma}^{ij}\tilde{D}_j\phi = 0 \tag{4.46}$$

As a reference, we give the Lichnerowicz equation (Hamiltonian constraint in terms of the conformal variables) for 4∂ST theories:

$$
\begin{aligned}
0 \;=\;& \tilde{\gamma}^{kl}\tilde{D}_k\tilde{D}_l\psi - \frac{1}{8}\psi\left(R[\tilde{D}] - \frac{1}{2}\tilde{\gamma}^{ij}\partial_i\phi\partial_j\phi\right) \\
& -\psi^5\left(\frac{1}{12}K^2 - \frac{1}{8}V(\phi)\right) + \frac{1}{8}\psi^{-7}\left(\tilde{A}_{kl}\tilde{A}^{kl} + 2\tilde{K}_\phi^2\right) \\
& +\frac{1}{8}\epsilon_1 f_1(\phi)\psi^5\left(12\psi^{-24}\tilde{K}_\phi^4 - 2\psi^{-16}\tilde{K}_\phi^2\tilde{\gamma}^{ij}\partial_i\phi\partial_j\phi - \frac{1}{4}\psi^{-8}(\tilde{\gamma}^{ij}\partial_i\phi\partial_j\phi)^2\right) \\
& +\frac{1}{4}\epsilon_2\psi^{-3}\Big[\tilde{D}_{i_3}\tilde{D}^{j_3}f_2(\phi) - 2\tilde{D}_{i_3}\ln\psi\tilde{D}^{j_3}f_2(\phi) - 2\tilde{D}_{i_3}f_2(\phi)\tilde{D}^{j_3}\ln\psi \\
& +2\tilde{\gamma}^{j_3}_{i_3}\tilde{\gamma}^{kl}\tilde{D}_k\ln\psi\tilde{D}_l f_2(\phi) - 2\psi^{-8}f_2'(\phi)\tilde{K}_\phi\tilde{A}_{i_3}{}^{j_3} - \frac{2}{3}\psi^{-2}f_2'(\phi)\tilde{K}_\phi K\tilde{\gamma}^{j_3}_{i_3}\Big] \\
& \times\Big(\gamma^{i_1i_2i_3}_{j_1j_2j_3}R[\tilde{D}]_{i_1i_2}{}^{j_1j_2} + 8\psi^{-1}\tilde{D}^{i_3}\tilde{D}_{j_3}\psi - 8\psi^{-1}\tilde{\gamma}^{i_3}_{j_3}\tilde{D}_k\tilde{D}^k\psi \\
& -24\psi^{-2}\tilde{D}^{i_3}\psi\tilde{D}_{j_3}\psi - 16\psi^{-2}\tilde{\gamma}^{i_3}_{j_3}\tilde{D}_k\psi\tilde{D}^k\psi + \frac{4}{9}\psi^4K^2\tilde{\gamma}^{i_3}_{j_3} \\
& -\frac{4}{3}\psi^{-2}K\tilde{A}^{i_3}_{j_3} + 4\psi^{-8}\tilde{A}^{i_3}{}_k\tilde{A}^k{}_{j_3} - 2\psi^{-8}\tilde{A}^k{}_l\tilde{A}^l{}_k\tilde{\gamma}^{i_3}_{j_3}\Big)
\end{aligned} \tag{4.47}
$$

Similarly, one can write the momentum constraint using the CTT variables

$$
\begin{aligned}
0 \;=\;& \tilde{\Delta}_L Y^i - \frac{2}{3}\psi^6\tilde{\gamma}^{ij}\tilde{D}_jK - \tilde{K}_\phi\left(1 + 2\epsilon_1 f_1(\phi)X\right)\tilde{\gamma}^{ij}\tilde{D}_j\phi \\
& +4\epsilon_2\psi^{-4}\gamma^{ii_1i_2}_{jj_1j_2}\Big[\tilde{D}_{i_2}\tilde{D}^{j_2}f_2(\phi) - 2\tilde{D}_{i_2}\ln\psi\tilde{D}^{j_2}f_2(\phi) - 2\tilde{D}_{i_2}f_2(\phi)\tilde{D}^{j_2}\ln\psi \\
& +2\tilde{\gamma}^{j_2}_{i_2}\tilde{\gamma}^{kl}\tilde{D}_k\ln\psi\tilde{D}_l f_2(\phi) - 2\psi^{-8}f_2'(\phi)\tilde{K}_\phi\tilde{A}_{i_2}{}^{j_2} - \frac{2}{3}\psi^{-2}f_2'(\phi)\tilde{K}_\phi K\gamma^{j_2}_{i_2}\Big] \\
& \times\left(\tilde{D}^j\tilde{A}_{i_1}{}^{j_1} + \frac{1}{3}\tilde{\gamma}^{j_1}_{i_1}\psi^6\tilde{D}^jK - 4\tilde{A}^{j_1}_{i_1}\tilde{D}^j\ln\psi - 2\tilde{\gamma}^{j_1}_{i_1}\tilde{A}^{jl}\tilde{D}_l\ln\psi\right) \\
& +\epsilon_2\psi^{-4}\left[\tilde{A}_k{}^j\tilde{D}^kf_2(\phi) + \frac{1}{3}\psi^6K\tilde{D}^jf_2(\phi) - \psi^6\tilde{D}^j\left(f_2'(\phi)\psi^{-6}\tilde{K}_\phi\right)\right] \\
& \times\Big(\gamma^{ii_1i_2}_{jj_1j_2}R[\tilde{D}]_{i_1i_2}{}^{j_1j_2} + 8\psi^{-1}\tilde{D}_i\tilde{D}^j\psi - 8\psi^{-1}\tilde{\gamma}^i_j\tilde{D}_k\tilde{D}^k\psi \\
& -24\psi^{-2}\tilde{D}_i\psi\tilde{D}^j\psi - 16\psi^{-2}\tilde{\gamma}^i_j\tilde{D}_k\psi\tilde{D}^k\psi + \frac{4}{9}\psi^4K^2\tilde{\gamma}^i_j \\
& -\frac{4}{3}\psi^{-2}K\tilde{A}^i_j + 4\psi^{-8}\tilde{A}^{ik}\tilde{A}_{kj} - 2\psi^{-8}\tilde{A}^{kl}\tilde{A}_{kl}\tilde{\gamma}^i_j\Big)
\end{aligned} \tag{4.48}
$$

where one has to convert $\tilde{A}^{ij}$ to the variables $\tilde{A}_{\rm TT}$, Y^i using (4.18)-(4.20). As explained in the subsequent sections, despite the length and lack of elegance of the equations, it is quite simple to extend the existence and uniqueness theorems of section 4.2.2 to equations (4.47)-(4.48), at least for small couplings. In particular, numerical relativists should not be discouraged after seeing these equations: at weak coupling they can be solved iteratively, starting from a GR solution.

4.2.5 Existence and uniqueness in scalar-tensor effective field theories

In this section we establish a well-posedness result for the elliptic boundary value problem of the CTT formulation of the 4∂ST constraints. We start by recalling the implicit function theorem in Banach spaces (see e.g. [112]).

Theorem 4.6 (Implicit function theorem in Banach spaces)**.** *Let $\mathcal{B}_x$, $\mathcal{B}_y$ and $\mathcal{B}_z$ be Banach spaces and let $\mathcal{F}$ be a C^1 (in the sense of Fréchet derivatives) map $\mathcal{B}_x \times \mathcal{B}_y \to \mathcal{B}_z$ such that $\mathcal{F}(x_0, y_0) = 0$ for some $(x_0, y_0) \in \mathcal{B}_x \times \mathcal{B}_y$ and the Fréchet derivative $y \mapsto \mathcal{D}_y\mathcal{F}|_{(x_0,y_0)}(0, y)$ is an isomorphism $\mathcal{B}_y \to \mathcal{B}_z$. Then there exists a neighbourhood $\Omega \subset \mathcal{B}_x$ of x_0 and a unique C^1 map $\mathcal{G} : \Omega \to \mathcal{B}_y$ such that $\mathcal{G}(x_0) = y_0$ and $\mathcal{F}(x, \mathcal{G}(x)) = 0$ for every $x \in \Omega$.*

It is perhaps worth going on a small detour and reviewing the main idea of the proof of this theorem. Let us denote the Fréchet derivative (i.e. "linearization") of the functional $\mathcal{F}$ at (x_0, y_0) by $\mathcal{A}$. Note that $\mathcal{A}$ is a linear operator $\mathcal{B}_y \to \mathcal{B}_z$ and an isomorphism by assumption. The equation $\mathcal{F}(x, y) = 0$ can be rewritten as

$$\mathcal{A}y = \mathcal{R}(x, y) \qquad \text{or} \qquad y = \mathcal{A}^{-1}\mathcal{R}(x, y) \tag{4.49}$$

with

$$\mathcal{R}(x, y) \equiv \mathcal{A}y - \mathcal{F}(x, y). \tag{4.50}$$

It can be shown that there is an open ball in $\mathcal{B}_x$ centered around x_0 such that for a fixed x the map $\mathcal{A}^{-1}\mathcal{R}(x, \cdot) : \mathcal{B}_y \to \mathcal{B}_y$ is a contraction map. The theorem then follows by the Banach fixed point theorem, i.e. there is a unique solution y to the equation $y = \mathcal{A}^{-1}\mathcal{R}(x, y)$ near y_0. The practical importance of the fact that $\mathcal{A}^{-1}\mathcal{R}(x, y)$ is a contraction map is that the equation can be solved by iterations.

To state and prove a theorem on the 4∂ST constraints, we need to make use of a few standard results on elliptic operators in asymptotically Euclidean manifolds [108]. Let $(\Sigma, \tilde{\gamma})$ be an n-dimensional asymptotically Euclidean manifold of class $W^p_{s,\delta}$ with

$$n - 2 - \frac{n}{p} > \delta > -\frac{n}{p}, \qquad\qquad p > \frac{n}{2}. \tag{4.51}$$

To apply the implicit function theorem to the nonlinear 4∂ST constraints, one needs to study the linearization of these equations. The first lemma will be used for the discussion of the linearized Lichnerowicz equation.

Lemma 4.2. *Consider a* $W^p_{s-2,\delta+2}$ *scalar function* c *on* Σ *and define the Poisson operator*

$$L_P : u \mapsto \tilde{\gamma}^{kl} \tilde{D}_k \tilde{D}_l u - cu$$

for a $W^p_{s,\delta}$ *scalar function* u *on* Σ*. Assume furthermore that* (4.51) *and one of the following two hypotheses holds*

1) $c \geq 0$ *and* $s > 2 + \frac{n}{p}$
2) $s \geq 2$ *and for any nontrivial* $f \in W^p_{s,\delta}(\Sigma)$

$$\int_\Sigma d^n \sqrt{\tilde{\gamma}} \left(\tilde{\gamma}^{ij} \partial_i f \partial_j f + c f^2 \right) > 0 \tag{4.52}$$

Then the operator L_P *is an isomorphism* $W^p_{s,\delta}(\Sigma) \to W^p_{s-2,\delta+2}(\Sigma)$*, i.e. the unique* $W^p_{s,\delta}$ *solution of the equation* $L_P u = 0$ *is* $u \equiv 0$*.*

A similar result will be required for the linearized momentum constraint which comes down to a statement on the conformal vector Laplacian (4.22) [90].

Lemma 4.3. *On our* n*-dimensional asymptotically Euclidean manifold* $(\Sigma, \tilde{\gamma})$ *of class* $W^p_{s,\rho}$*, let us assume the inequalities* (4.51)*.*

(1) *The kernel of the conformal Laplace operator* Δ_L *is the space of conformal Killing vector fields of* $(\Sigma, \tilde{\gamma})$*.*

(2) *The manifold* $(\Sigma, \tilde{\gamma})$ *has no conformal Killing vector fields of class* $W^p_{s,\delta}$ *under the above assumptions. Therefore,* Δ_L *is an isomorphism* $W^p_{s,\delta}(\Sigma) \to W^p_{s-2,\delta+2}(\Sigma)$*.*

Of course, the initial data slice $(\Sigma, \tilde{\gamma})$ can have e.g. smooth conformal Killing vector fields, it is simply growth at infinity that rules out the possibility of a conformal Killing vector field that is weighted Sobolev regular with the above requirements.

Finally, we are in the position to combine all these results to a theorem on the conformally formulated 4∂ST constraints.

Theorem 4.7. *Let $(\Sigma, \tilde{\gamma})$ be an 3-dimensional asymptotically Euclidean manifold of type $W^p_{s,\delta}$ with*

$$p > \frac{3}{2}, \qquad s > 2 + \frac{3}{p} \qquad \text{and} \qquad \frac{1}{2} - \frac{3}{p} < \delta < 1 - \frac{3}{p}.$$

Assume that we are given a solution of the CTT Einstein-scalar-field constraint equations (ψ_0, Y_0) with $\psi_0 > 0$ and $\psi_0 - 1, Y_0 \in W^p_{s,\delta}(\Sigma)$ corresponding to free data $(\tilde{\gamma}, K, \tilde{A}_{TT}, \phi, \tilde{K}_\phi)$. Our hypothesis on the free data is $\phi - \phi_\infty \in W^p_{s,\delta}(\Sigma)$ where ϕ_∞ is the asymptotic (constant) value of the scalar field, $V(\phi) \in W^p_{s-2,\delta+2}(\Sigma)$, $\tilde{A}_{TT}, \tilde{K}_\phi \in W^p_{s-1,\delta+1}(\Sigma)$ and $K = 0$.

Then the 4∂ST constraint system (4.47)-(4.48) admits a unique solution (ψ, Y) for sufficiently small values of ϵ_1 and ϵ_2 with the same free data, provided that

(i) $f_1(\phi) - f_1(\phi_\infty), f_2(\phi) - f_2(\phi_\infty) \in W^p_{s,\delta}(\Sigma)$ *and*

(ii) for every non-trivial function $f \in W^p_{2,\rho}(\Sigma)$ with $\rho > \frac{1}{2} - \frac{3}{p}$ the following inequality holds:

$$\int_\Sigma d^n x \sqrt{\tilde{\gamma}} \left[\tilde{\gamma}^{ij} \partial_i f \partial_j f + c f^2\right] > 0 \tag{4.53}$$

with

$$c \equiv \frac{1}{8}\left(R[\tilde{D}] + 7\psi_0^{-8} \tilde{A}_{kl} \tilde{A}^{kl} + 14\psi_0^{-6} \tilde{K}_\phi^2 - \frac{1}{2}\tilde{\gamma}^{ij}\partial_i\phi\partial_j\phi - 5\psi_0^4 V(\phi)\right)$$

The 4∂ST solution (ψ, Y) is near the Einstein-scalar-field solution in the sense of $W^p_{s,\delta}$ norms.

Proof. The result follows by a straightforward application of the implicit function theorem. Take

$$x \equiv \Big(\epsilon_1 f_1(\phi), \epsilon_2 f_2(\phi)\Big), \qquad y \equiv (\psi, Y), \qquad z \equiv \Big(\mathcal{H}(x, y), \mathcal{M}(x, y)\Big) \tag{4.54}$$

with

$$\mathcal{B}_x \equiv W^p_{s,\delta}(\Sigma) \times W^p_{s,\delta}(\Sigma), \qquad \mathcal{B}_y = W^p_{s,\delta}(\Sigma) \times W^p_{s,\delta}(\Sigma) \tag{4.55}$$

The next step is to use the Sobolev multiplication properties (Lemma 4.1) together with the assumptions on s and δ to check that the 4∂ST Hamiltonian and momentum constraints (4.47)-(4.48) map into

$$\mathcal{B}_z \equiv W^p_{s-2,\delta+2}(\Sigma) \times W^p_{s-2,\delta+2}(\Sigma) \tag{4.56}$$

To see this, we first note that the m^{th} derivatives of a tensor field of class $W^p_{s,\delta}$ are of class $W^p_{s-m,\delta+m}$. Taking $s_1 = s_2 = s-1$, $s_3 = s-2$, $\delta_1 = \delta_2 = \delta+1$ and $\delta_3 = \delta+2$ in Lemma 4.1, we find that pointwise multiplication of two tensor fields of class $W^p_{s-1,\delta+1}$ is of class $W^p_{s-2,\delta+2}$. Similarly, with $s > 2+3/p$ and $\delta > -3/p$, pointwise multiplication satisfies

$$\begin{aligned} W^p_{s-2,\delta+2}(\Sigma) \times W^p_{s,\delta}(\Sigma) &\to W^p_{s-2,\delta+2}(\Sigma) \\ W^p_{s-2,\delta+2}(\Sigma) \times W^p_{s-2,\delta+2}(\Sigma) &\to W^p_{s-2,\delta+2}(\Sigma) \\ W^p_{s-2,\delta+2}(\Sigma) \times W^p_{s,\delta}(1,\Sigma) &\to W^p_{s-2,\delta+2}(\Sigma) \end{aligned}$$

Since each term in (4.47)-(4.48) can be written as a product of terms in one of $W^p_{s,\delta}$, $W^p_{s-1,\delta+1}$ or $W^p_{s-2,\delta+2}$, it follows that the constraints map into $\mathcal{B}_z$.

To apply the implicit function theorem, take the point $x_0 \in \mathcal{B}_x$ to be $x_0 = (0,0)$ (corresponding to vanishing EFT couplings), and $y_0 = (\psi_0, Y_0)$ to be the solution of the constraints of the $\epsilon_1 = \epsilon_2 = 0$ theory with the given free data (which exists by assumption). The Fréchet derivative at (x_0, y_0) is obtained by linearizing (4.47)-(4.48) in the variables (ψ, Y) at $\epsilon_1 = \epsilon_2 = 0$. Its action on the element $(0, y)$ with $y \equiv (\delta\psi, \delta Y)$ is just the linear elliptic operator

$$\mathcal{D}_y\mathcal{F}(0;\delta\psi,\delta Y) = \begin{pmatrix} \tilde{\gamma}^{kl}\tilde{D}_k\tilde{D}_l - c & \frac{1}{4}\psi_0^{-7}\tilde{A}_{kl}(\tilde{L}\cdot)^{kl} \\ 0 & \tilde{\Delta}_L \end{pmatrix} \begin{pmatrix} \delta\psi \\ \delta Y \end{pmatrix} \tag{4.57}$$

Lemma 4.2 tells us that the Poisson operator $\tilde{\gamma}^{kl}\tilde{D}_k\tilde{D}_l - c$ is an isomorphism if for every non-trivial function $f \in W^p_{2,\rho}(\Sigma)$ (with $\rho > \frac{1}{2} - \frac{3}{p}$) the inequality (4.53) is satisfied which is true by assumption.

Moreover, $\tilde{\Delta}_L$ is also an isomorphism on asymptotically Euclidean manifolds due to Lemma 4.3. Since $\mathcal{D}_y\mathcal{F}$ is upper triangular and the operators in the diagonals are isomorphisms, it follows that $\mathcal{D}_y\mathcal{F}$ is also an isomorphism. Therefore, the assumptions of the implicit function theorem are satisfied which concludes the proof. □

We conclude this subsection by a short discussion of how the inequality (4.53) applies to the construction of initial data for a binary system of black holes with scalar hair. We first note that if $V(\phi) \geq 0$ then the minimally coupled scalar obeys the dominant energy condition. Furthermore, on a maximal slice $R[D] = K_{ij}K^{ij} + \varrho + 4\partial\text{ST corrections} \geq 0$ which implies that the metric γ is in the positive Yamabe class. By virtue of the conformal invariance of the functional $I_\gamma[f]$ (defined in (4.28)), $\tilde{\gamma}$ is also in the positive Yamabe class. Astrophysically relevant stationary black hole solutions in a weakly coupled 4∂ST theory are expected to have only a small amount of scalar hair. The reason for this is that there are no known stable scalar hairy black hole solutions in the $\epsilon_1 = \epsilon_2 = 0$ theory. Therefore, the functional in (4.53) is expected to be positive for scalar hairy black hole data, as well as scalar hairy black hole binary data.

4.2.6 Construction of puncture data for scalar-tensor EFT

The fact that the momentum constraint has such a simple form when written in terms of the conjugate momenta has the remarkable consequence that one can straightforwardly generalize the Bowen-York-type approach to a more general class of theories. The solution to the momentum constraint with N punctures located at $c_{(\alpha)}$ is given by

$$\tilde{\gamma}_{ij} = \delta_{ij}, \qquad \tilde{\pi}_\phi = 0, \qquad \tilde{\pi}^{ij} = B^{ij} \tag{4.58}$$

where the traceless Bowen-York tensor B^{ij} is given by

$$\begin{aligned} B^{ij} \; &= \sum_{\alpha=1}^{N} \Bigg[\frac{3}{2r_{(\alpha)}^2} \left(P^i_{(\alpha)} \hat{x}^j_{(\alpha)} + P^j_{(\alpha)} \hat{x}^i_{(\alpha)} - \left(\delta^{ij} - \hat{x}^i_{(\alpha)} \hat{x}^j_{(\alpha)} \right) P_k \hat{x}^k_{(\alpha)} \right) \\ &\quad + \frac{3}{r_{(\alpha)}^3} \left(\epsilon^i{}_{kl} S^k_{(\alpha)} \hat{x}^l_{(\alpha)} \hat{x}^j_{(\alpha)} + \epsilon^j{}_{kl} S^k_{(\alpha)} \hat{x}^l_{(\alpha)} \hat{x}^i_{(\alpha)} \right) \Bigg] \end{aligned} \tag{4.59}$$

with $r_{(\alpha)} \equiv |x - c_{(\alpha)}|$ and $\hat{x}_{(\alpha)} \equiv \left(x - c_{(\alpha)} \right) / r_{(\alpha)}$. Note that we have not specified the initial scalar field configuration yet, (4.58) is a solution regardless of what $\phi(x)$ is.

For the moment, assume that we are given a suitably regular (specified later) initial data for ϕ. Furthermore, as in section 4.2.3, it is useful to write the conformal factor as a sum of a singular piece and a regular piece u:

$$\psi = 1 + \frac{1}{\mu} + u, \qquad \frac{1}{\mu} \equiv \sum_{\alpha=1}^{N} \frac{m_{(\alpha)}}{2r_{(\alpha)}} \tag{4.60}$$

Then, to obtain initial data for the variables u, K_ϕ and $K^i{}_j$ (or equivalently, for ψ, K, $\tilde{A}_{ij}$, $\tilde{K}_\phi$), one needs to solve the system of equations consisting of the elliptic PDE

$$\begin{aligned}
0 \;=\;& \partial^i\partial_i u + \frac{1}{16}\psi\partial_i\phi\partial^i\phi - \frac{1}{8}\psi^5\left(\delta^{i_1 i_2}_{j_1 j_2}K_{i_1}{}^{j_1}K_{i_2}{}^{j_2} - V(\phi) - 2K_\phi^2\right) \\
&+\frac{1}{8}\epsilon_1 f_1(\phi)\psi^5\left(12K_\phi^4 - 2\psi^{-4}K_\phi^2\,\partial_i\phi\partial^i\phi - \frac{1}{4}\psi^{-8}(\partial_i\phi\partial^i\phi)^2\right) \\
&+\frac{1}{4}\epsilon_2\psi^{-3}\Bigg(\partial_{i_3}\partial^{j_3}f_2(\phi) - 2\partial_{i_3}\ln\psi\;\partial^{j_3}f_2(\phi) - 2\partial_{i_3}f_2(\phi)\partial^{j_3}\ln\psi \\
&+2\delta^{j_3}_{i_3}\partial^k\ln\psi\;\partial_k f_2(\phi) - 2\psi^4 f_2'(\phi)K_\phi K_{i_3}{}^{j_3}\Bigg) \\
&\times\Bigg(8\psi^{-1}\partial^{i_3}\partial_{j_3}\psi - 8\psi^{-1}\delta^{i_3}_{j_3}\partial_k\partial^k\psi - 24\psi^{-2}\partial^{i_3}\psi\;\partial_{j_3}\psi \\
&-16\psi^{-2}\delta^{i_3}_{j_3}\partial_k\psi\;\partial^k\psi + 2\psi^4\delta^{i_1 i_2 i_3}_{j_1 j_2 j_3}K^{j_1}_{i_1}K^{j_2}_{i_2}\Bigg)
\end{aligned} \tag{4.61}$$

and the set of algebraic equations (that come from the combination of (4.58), (4.41) and (4.42))

$$0 \;=\; -2K_\phi(1+2\epsilon_1 f_1(\phi)X) - \frac{4}{3}\epsilon_2 f_2'(\phi)\delta^{i_1 i_2 i_3}_{j_1 j_2 j_3}K_{i_1}{}^{j_1}K_{i_2}{}^{j_2}K_{i_3}{}^{j_3} \tag{4.62}$$

$$\begin{aligned}
\psi^{-6}B^i{}_j \;=\;& \delta^{ii_1}_{jj_1}K_{i_1}{}^{j_1} + 4\epsilon_2\delta^{ii_1i_2}_{jj_1j_2}K_{i_1}{}^{j_1}\Bigg[\psi^{-4}\partial_{i_2}\partial^{j_2}f_2(\phi) - f_2'(\phi)K_\phi K_{i_2}{}^{j_2} \\
&-2\psi^{-4}\partial_k f_2(\phi)\left(\delta^k_{i_2}\partial^{j_2}\ln\psi + \delta^{j_2 k}\partial_{i_2}\ln\psi - \delta^{j_2}_{i_2}\partial^k\ln\psi\right)\Bigg]
\end{aligned} \tag{4.63}$$

In the next subsection, it will be shown that this system of equations has a unique solution for small couplings (i.e. the couplings satisfy (4.44) with Λ taken to be the smallest of the bare masses) such that $u \in C^2(\mathbb{R}^3)$ and $K_\phi, K^i{}_j \in C^1(\mathbb{R}^3)$.

Several remarks are in order about this construction. First of all, note the placing of the indices in equations (4.62)-(4.63). The main reason for writing these equations in this particular form (apart from compactness) is that $K^i{}_j$ turns out to be regular on the entire initial slice (see next section for details), whereas K_{ij} is singular at the punctures.

Another natural question to ask is how to solve the system in practice. The most straightforward approach is to start with the puncture data of vacuum GR $\psi = \psi_0$, $K_\phi = 0$, $K_{ij} = \psi_0^{-2}B_{ij}$ and solve the system iteratively. At weak coupling, it seems likely that such an approach would converge quickly and the required number of iteration steps is fairly small.

It is also worth mentioning that the initial data described above inherits the appealing property of the original Bowen-York data that a single linear momentum source (i.e. the solution with $N = 1$, $P^i_{(1)} \neq 0$ and $S^i_{(1)} = 0$) has ADM momentum

$$P^i_{\text{ADM}} = \frac{1}{8\pi} \int\limits_{S_\infty} \mathrm{d}A\ \pi^{ij} \hat{x}_j = \frac{1}{8\pi} \int\limits_{S_\infty} \mathrm{d}A\ B^{ij} \hat{x}_j = P^i_{(1)}, \tag{4.64}$$

and a single angular momentum source (the solution with $N = 1$, $P^i_{(1)} = 0$ and $S^i_{(1)} \neq 0$)

$$J^i = \frac{1}{8\pi} \int\limits_{S_\infty} \mathrm{d}A\ \pi_{jk} \epsilon^{ijl} x_l \hat{x}^k = \frac{1}{8\pi} \int\limits_{S_\infty} \mathrm{d}A\ B_{jk} \epsilon^{ijl} x_l \hat{x}^k = S^i_{(1)}, \tag{4.65}$$

respectively, as expected.

Now let us address the question of how to choose initial data for the scalar field. Unfortunately, there appears to be no natural choice of the initial $\phi(x)$ that could be written down in a simple closed form. Of course, one could approximate the initial value of ϕ with a superposition of a set of scalar cloud configurations localised around the punctures, multiplied by some regularizing function that satisfies the regularity conditions stated in the next section. But such data is likely to contain significant junk scalar radiation in addition to the junk gravitational radiation already present in the GR version of the puncture data.

There is another possible caveat with this construction. Suppose that one evolves this initial data e.g. by solving the modified harmonic gauge equations of motion of the theory. Then even after a small amount of time the fields may become strong in the interior of the black holes (or perhaps in the exterior as well, if the black holes are not large enough), leading to a breakdown of strong hyperbolicity of the evolution equations. However, this issue may be resolved by excising the interior of the black holes and solve the equations in the exterior. This would require imposing boundary conditions on the excision boundary. Hence for N black holes it may be better to set up initial data by solving the constraint equations on e.g. $\mathbb{R}^3$ minus N balls and impose apparent horizon boundary conditions on the boundaries of the balls (see section 4.4).

4.2.7 Existence and uniqueness of puncture data for scalar-tensor effective field theory

Now we demonstrate that the construction just described yields a unique initial data for the variables ψ and $K_I \equiv (K_\phi, K^i{}_j)$, provided we are given $W^p_{s,\delta}(\mathbb{R}^3)$ data for ϕ subject to some extra requirements at the punctures. For notational convenience, let $\Pi_I \equiv (\pi_\phi, \pi^i{}_j - \psi^{-6}B^i{}_j)$. We proceed very similarly as in section 4.2.5: we define a map $z \equiv \mathcal{F}(x, y)$ with

$$x \equiv \Big(\epsilon_1 f_1(\phi), \epsilon_2 f_2(\phi)\Big), \qquad y \equiv (u, K_I), \qquad z \equiv \Big(\mathcal{H}(x,y), \Pi_I(x,y)\Big) \tag{4.66}$$

with

$$\mathcal{B}_x \equiv W^p_{3,\delta}(\mathbb{R}^3) \times W^p_{3,\delta}(\mathbb{R}^3), \qquad \mathcal{B}_y = W^p_{3,\delta}(\mathbb{R}^3) \times W^p_{2,\delta+1}(\mathbb{R}^3) \tag{4.67}$$

To cancel the singularities of ψ and make the Einstein-scalar-field and 4∂ST terms regular in (4.61), we have to assume $\lim\limits_{r_{(\alpha)}\to 0} r_{(\alpha)}^{-1/2}\partial_i\phi = 0$ and $\lim\limits_{r_{(\alpha)}\to 0} r_{(\alpha)}^{-5}V(\phi) = 0$. There is no such problem with the rest of the terms in (4.61) since they are multiplied by negative powers of the conformal factor. Now let $s \geq 3$ and $p > 3$ which implies $\phi \in C^2(\mathbb{R}^3)$. Assuming $f_1(\phi), f_2(\phi) \in W^p_{s,\delta}(\mathbb{R}^3)$ and $V(\phi) \in W^p_{s-2,\delta+2}(\mathbb{R}^3)$, the Sobolev multiplication properties (Lemma 4.1) imply

$$\mathcal{B}_z \equiv W^p_{1,\delta+2}(\mathbb{R}^3) \times W^p_{2,\delta+1}(\mathbb{R}^3) \tag{4.68}$$

Note that in this case $\mathcal{F}(x, y) = 0$ is an elliptic PDE for u coupled to a set of algebraic equations for K_I. Take $x_0 = 0$ (i.e. $\epsilon_1 = \epsilon_2 = 0$) and let y_0 denote the original Bowen-York solution $y_0 \equiv (u_0, K_{I0}) \in \mathcal{B}_y$ described in section 4.2.3. We wish to use the implicit function theorem to show that for small enough couplings, the equations (4.61)-(4.62) admit a unique solution. To do this, we compute the action of $\mathcal{D}_y\mathcal{F}$ at (x_0, y_0) acting on the element $(0, y)$ with $y \equiv (\delta u, \delta K_I)$. Let us denote the components of $\mathcal{D}_y\mathcal{F}\Big|_{(x_0,y_0)}(0, y)$ by $\left(\delta\mathcal{H}, \delta\pi_\phi, \delta\pi^i{}_j\right)^T$. Then we have

$$\begin{pmatrix} \delta\mathcal{H} \\ \delta\pi_\phi \\ \delta\pi^i{}_j \end{pmatrix} = \begin{pmatrix} \tilde{\gamma}^{kl}\tilde{D}_k\tilde{D}_l - \frac{7}{8}\psi_0^{-8}B_{kl}B^{kl} & 0 & \frac{1}{4}\psi_0^{-1}B^l{}_k \\ 0 & 2 & 0 \\ 0 & 0 & \delta^{il}_{jk} \end{pmatrix} \begin{pmatrix} \delta u \\ \delta K_\phi \\ \delta K^k{}_l \end{pmatrix} \tag{4.69}$$

which is clearly invertible (due to Lemma 4.2) and thus the map $\mathcal{F}$ obeys the conditions of Theorem (4.6). Therefore, we have the following result.

Theorem 4.8 (Existence and uniqueness of puncture data). *Let $\phi \in W^p_{s,\delta}(\mathbb{R}^3)$ such that $s \geq 3$, $p > 3$ and $0 \leq \delta < 1 - \frac{3}{p}$. Then the system* (4.61)-(4.63) *admits a unique solution in the neighbourhood of the original puncture solution of section 4.2.3 for small enough ϵ_1, ϵ_2. The solution for the conformal factor ψ is of the form* (4.60) *with $u \in W^p_{3,\delta}(\mathbb{R}^3)$ and $K_\phi, K^i{}_j \in W^p_{2,\delta+1}(\mathbb{R}^3)$, provided that*

(i) $\lim_{r_{(\alpha)} \to 0} r_{(\alpha)}^{-1/2}\, \partial_i \phi = 0$ *and* $\lim_{r_{(\alpha)} \to 0} r_{(\alpha)}^{-5}\, V(\phi) = 0.$

(ii) $f_1(\phi) - f_1(\phi_\infty), f_2(\phi) - f_2(\phi_\infty) \in W^p_{3,\delta}(\mathbb{R}^3)$ *and* $V(\phi) \in W^p_{1,\delta+2}(\mathbb{R}^3)$

Moreover, $u \in C^2(\mathbb{R}^3)$ and $K_\phi, K^i{}_j \in C^1(\mathbb{R}^3)$.

Note that assumption (i) may be dropped if the constraints are solved on an excised initial data surface, such as $\mathbb{R}^3$ minus N balls.

4.3 The conformal thin sandwich method

4.3.1 The conformal thin sandwich equations

An alternative but closely related way to construct asymptotically Euclidean initial data is the so-called conformal thin sandwich (CTS) method, originally proposed by York [101]. The mathematical formulation of the method only slightly differs from the CTT approach but the difference is important from a physics point of view: the CTS version provides a more natural way to prepare initial data that is nearly stationary. This is an improvement compared to the Bowen-York data in the sense that one can significantly reduce the amount of junk radiation plaguing the initial stages of a numerical simulation. However, there is a cost to pay for this: to achieve such data, one has to solve the momentum constraint, as well as the Hamiltonian constraint using an elliptic solver.

Once again, our starting point is the conformal metric (4.9) and the decomposition of the extrinsic curvature (4.10). The main difference compared to the CTT approach is the further treatment of the variable $\tilde{A}_{ij}$. Let α denote the lapse function and β^i the shift vector. Then introducing[3]

$$U^{ij} \equiv (\det \tilde{\gamma})^{-1/3} \partial_t \left[\tilde{\gamma}^{ij} (\det \tilde{\gamma})^{1/3} \right] \qquad \text{and} \qquad \tilde{\alpha} \equiv \psi^{-6} \alpha, \tag{4.70}$$

[3]In some numerical relativity applications the conformal metric is chosen such that $\det \tilde{\gamma} = 1$ and in that case $U^{ij} = \partial_t \tilde{\gamma}^{ij}$.

allows us to write

$$\tilde{A}^{ij} = \frac{1}{2\tilde{\alpha}}\left[(\tilde{L}\beta)^{ij} + U^{ij}\right] \tag{4.71}$$

where the conformal Killing operator $\tilde{L}$ was defined in (4.20). Thus in the CTS decomposition the variables U^{ij} and β^i are used instead of the CTT variables $\tilde{A}^{ij}_{\mathrm{TT}}$ and Y^i. Plugging (4.71) into the Hamiltonian and momentum constraints (4.5)-(4.6) of general relativity gives elliptic equations for the variables (ψ, β^i), whereas the 'free data' now consists of the sextuple $(\tilde{\alpha}, \tilde{\gamma}_{ij}, U^{ij}, K, \tilde{\varrho}, \tilde{\mathfrak{p}}^i)$. Therefore, the CTS constraints can be written as

$$\tilde{\gamma}^{kl}\tilde{D}_k\tilde{D}_l\psi - \frac{1}{8}\psi R[\tilde{D}] - \frac{1}{12}\psi^5 K^2 + \frac{1}{8}\psi^{-7}\tilde{A}_{kl}\tilde{A}^{kl} + \frac{1}{8}\psi^{-3}\tilde{\varrho} \quad = 0 \tag{4.72}$$

$$\tilde{D}_j\tilde{A}^{ij} - \frac{2}{3}\psi^6\tilde{\gamma}^{ij}\tilde{D}_jK - \frac{1}{2}\tilde{\mathfrak{p}}^i \quad = 0. \tag{4.73}$$

where $\tilde{A}$ is to be replaced by the RHS of (4.71). As mentioned, this system has very similar properties as the CTT system. In particular, given suitable free data, a unique solution exists to the corresponding elliptic boundary value problem under very similar conditions. Moreover, the Hamiltonian constraint decouples from the momentum constraint on CMC slices as in the case of the CTT system.

Consider now the scalar-tensor theory (1.5) at weak coupling. The CTS equations for this theory can be obtained in exactly the same way: i.e., by substituting the decomposition (4.71) into (4.47)-(4.48). For small enough ϵ_1 and ϵ_2, this is an elliptic PDE system for (ψ, β^i). In the next section, we state a well-posedness theorem for the corresponding elliptic boundary value problem.

4.3.2 Mathematical statements

The similarity of the CTT and CTS equations allows us to straightforwardly transform statements about one of these systems to statements about the other one. The only extra requirement we need concerns the conformal lapse function $\tilde{\alpha}$. It is customary to choose the lapse so that its asymptotic value at spatial infinity approaches 1. Hence, the natural assumption on $\tilde{\alpha}$ (which is part of the free data) is $\tilde{\alpha} \in W^p_{s,\delta}(1, \Sigma)$ (defined in (4.25)) and $\tilde{\alpha} > 0$. Then the methods used to obtain Theorem 4.5 imply the following.

Theorem 4.9. *Let (Σ, γ) be a 3-dimensional asymptotically Euclidean manifold of class $W^p_{s,\delta}$ with $K = 0$, $p > \frac{3}{2}$, $s > 2 + \frac{3}{p}$ and $1 - \frac{3}{p} > \delta > -\frac{3}{p}$. Moreover, suppose*

$$R[\tilde{D}] - \frac{1}{2}\tilde{\gamma}^{ij}\partial_i\phi\partial_j\phi > 0.$$

Then there exists an open set of values for the free data $(\tilde{\alpha}, U, \phi, \tilde{K}_\phi)$ *satisfying* $\tilde{\alpha} \in W^p_{s,\delta}(1,\Sigma)$, $\tilde{\alpha} > 0$, $\phi - \phi_\infty \in W^p_{s,\delta}(\Sigma)$, $U, \tilde{K}_\phi \in W^p_{s-1,\delta+1}(\Sigma)$ *and* $V(\phi) \in W^p_{s-2,\delta+2}(\Sigma)$ *such that the conformally formulated constraints have a solution* (ψ, β^i) *with* $\psi \in W^p_{s,\delta}(1,\Sigma)$, $\psi > 0$ *and* $\beta \in W^p_{s,\delta}(\Sigma)$.

Likewise, we have the CTS analogue of Theorem 4.7 for the 4-derivative scalar tensor theory (1.5). To avoid repetition, we only state this result without proof. (The proof is completely analogous to that of Theorem 4.7: it is a combination of the weighted Sobolev multiplication lemma and the implicit function theorem.)

Theorem 4.10. *Let* $(\Sigma, \tilde{\gamma})$ *be a* 3*-dimensional asymptotically Euclidean manifold of type* $W^p_{s,\delta}$ *with*

$$p > \frac{3}{2}, \qquad s > 3 + \frac{3}{p} \qquad \text{and} \qquad \frac{1}{2} - \frac{3}{p} < \delta < 1 - \frac{3}{p}.$$

Assume that we are given a solution of the CTS Einstein-scalar-field constraint equations (ψ_0, β^i_0) *with* $\psi_0 > 0$ *and* $\psi_0 - 1, \beta^i_0 \in W^p_{s,\delta}(\Sigma)$ *corresponding to free data* $(\tilde{\alpha}, \tilde{\gamma}, K, U, \phi, \tilde{K}_\phi)$ *satisfying* $\tilde{\alpha} \in W^p_{s,\delta}(1,\Sigma)$, $\tilde{\alpha} > 0$, $\phi - \phi_\infty \in W^p_{s,\delta}(\Sigma)$, $V(\phi) \in W^p_{s-2,\delta+2}(\Sigma)$, $\tilde{U}, \tilde{K}_\phi \in W^p_{s-1,\delta+1}(\Sigma)$ *and* $K = 0$.

Then the $4\partial ST$ *constraint system admits a unique solution* (ψ, β^i) *for small enough* ϵ_1, ϵ_2, *provided that* $f_1(\phi) - f_1(\phi_\infty), f_2(\phi) - f_2(\phi_\infty) \in W^p_{s,\delta}(\Sigma)$ *for every non-trivial function* $f \in W^p_{2,\rho}(\Sigma)$ *with* $\rho > \frac{1}{2} - \frac{3}{p}$ *the following inequality holds:*

$$\int_\Sigma d^n x \sqrt{\tilde{\gamma}} \left[\tilde{\gamma}^{ij} \partial_i f \partial_j f + c f^2 \right] > 0 \tag{4.74}$$

with

$$c \equiv \frac{1}{8} \left(R[\tilde{D}] + 7\psi_0^{-8} \tilde{A}_{kl} \tilde{A}^{kl} + 14\psi_0^{-6} \tilde{K}_\phi^2 - \frac{1}{2} \tilde{\gamma}^{ij} \partial_i \phi \partial_j \phi - 5\psi_0^4 V(\phi) \right)$$

The $4\partial ST$ *solution* (ψ, β^i) *is close to* (ψ_0, β^i_0) *in the sense of* $W^p_{s,\delta}(\Sigma)$ *norms.*

Similar results hold in the case when K is not identically but nearly zero and of class $W^p_{s-1,\delta+1}$ (which can be proved by using the implicit function theorem).

4.3.3 Choice of free data for black hole binaries

We end the discussion of the original conformal thin sandwich method by giving a brief account of how free data can be chosen for numerical simulations in general relativity and 4∂ST theories that approximates binary black hole systems.

In general relativity, a standard choice for the free data (for black hole binaries) is to take a "superposition" of two isolated Kerr solutions, with their respective coordinate origins shifted appropriately (see e.g. [113]). The idea is that as long as the separation of the two black holes is sufficiently large, the superposed geometry is a good first approximation of the actual geometry of the binary system. Then solving the constraints for (ψ, β^i) accounts for the deviation of this naive data from the actual binary black hole geometry. In more detail, let $\gamma^{(1)}_{ij}$, $\alpha^{(1)}$, $\beta^{(1)i}$, $\dot{\gamma}^{(1)}_{ij}$ be the induced metric, the lapse function, the shift vector and the time derivative of the induced metric, respectively, of the first Kerr black hole, written in a suitable coordinate system (usually Kerr-Schild coordinates). We use a similar notation for the second black hole. One can take the naive conformal metric and conformal lapse to be

$$
\begin{aligned}
\tilde{\gamma}_{ij} &= \gamma^{(1)}_{ij} + \gamma^{(2)}_{ij} - \delta_{ij} \\
\tilde{\alpha} &= \alpha^{(1)} + \alpha^{(2)} - 1
\end{aligned}
$$

and introduce an auxiliary shift vector defined by

$$
\beta^i_{\text{aux}} = \beta^{(1)i} + \beta^{(2)i}
$$

Inspired by the identities

$$
\begin{aligned}
U^{ij} &= \psi^4 \left(\partial_t \gamma^{ij} - \frac{1}{3} \gamma^{ij} \gamma_{kl} \partial_t \gamma^{kl} \right) \\
K &= \frac{1}{2\alpha} \left(\gamma_{ij} \partial_t \gamma^{ij} + 2 \partial_i \beta^i + \gamma^{ij} \beta^k \partial_k \gamma_{ij} \right)
\end{aligned}
$$

and taking $\psi_{aux} = 1$ as the naive approximate solution for the conformal factor, we can choose the rest of the free data as

$$
\begin{aligned}
U^{ij} &= -\tilde{\gamma}^{ik} \tilde{\gamma}^{jl} \left(U^{\text{aux}}_{kl} - \frac{1}{3} \tilde{\gamma}_{kl} \tilde{\gamma}^{mn} U^{\text{aux}}_{mn} \right) \qquad \text{with} \qquad U^{\text{aux}}_{ij} \equiv \dot{\gamma}^{(1)}_{ij} + \dot{\gamma}^{(2)}_{ij} \\
K &= \frac{1}{2\tilde{\alpha}} \left(\tilde{\gamma}_{ij} U^{ij} + 2 \partial_i \beta^i_{\text{aux}} + \tilde{\gamma}^{ij} \beta^k_{\text{aux}} \partial_k \tilde{\gamma}_{ij} \right)
\end{aligned}
$$

The construction just described works essentially the same way for the scalar-tensor theories (1.5). The only difference is that for a 4∂ST theory the gravitational part of the free data is constructed using a black hole solution of the theory which for generic couplings differs from the Kerr solution. The natural choice for the scalar part of the free data is to follow the philosophy of "superposition" and take

$$\phi = \phi^{(1)} + \phi^{(2)} - \phi_\infty, \qquad \dot{\phi} = \dot{\phi}^{(1)} + \dot{\phi}^{(2)} \tag{4.75}$$

where $\phi^{(1)}$, $\phi^{(2)}$ and $\dot{\phi}^{(1)}$, $\dot{\phi}^{(2)}$ are the scalar field configurations of the black holes and their time derivatives, ϕ_∞ is the asymptotic value of the scalar field at spatial infinity (which may be non-zero).

4.4 The extended conformal thin sandwich method

4.4.1 Quasiequilibrium initial data for general relativity

A proposal for initial data in GR representing a binary black hole system in quasiequilibrium is provided by an extension of the Conformal Thin Sandwich method [105].

The purpose of this approach is to construct initial data for two black holes moving along circular orbits. In other words, the binary system is assumed to be in quasiequilibrium, meaning that the spacetime possesses an approximate helical Killing vector field ξ_{hel} that generates circular orbits. Given such a vector field, one could choose coordinates which co-rotate with the binary system. This amounts to choosing a time coordinate such that $\partial/\partial t$ is parallel with ξ_{hel}. (Of course, with this choice $\partial/\partial t$ will not be timelike everywhere.) Then the requirement of quasiequilibrium can be expressed as $\partial_t g_{\mu\nu} \approx 0$. Using the conformal variables, one could set

$$\partial_t \tilde{\gamma}_{ij} = 0, \qquad \partial_t K = 0 \tag{4.76}$$

on the initial slice. The first of these two criteria implies

$$\tilde{A}^{ij} = \frac{\psi^6}{2\alpha} (\tilde{L}\beta)^{ij} \tag{4.77}$$

Substituting this into the momentum constraint yields

$$\tilde{\Delta}_L \beta^i - (\tilde{L}\beta)^{ij} \tilde{D}_j \ln(\psi^{-6}\alpha) = \frac{4}{3}\alpha \tilde{D}^i K \tag{4.78}$$

In the extended CTS approach one obtains an extra elliptic equation that involves the lapse function. To derive this equation, consider the following combination of the equations of motion

$$\frac{1}{4}\alpha\psi^5 \left(2\gamma^{\mu\nu} G_{\mu\nu} + \mathcal{H}\right) = 0 \tag{4.79}$$

The only second time derivative term in equation (4.79) is $\partial_t K$ so using (4.76) gives the constraint equation

$$\tilde{\gamma}^{ij}\tilde{D}_i\tilde{D}_j(\alpha\psi) = \alpha\psi\left(\frac{7}{8}\psi^{-8}\tilde{A}_{ij}\tilde{A}^{ij} + \frac{5}{12}\psi^4K^2 + \frac{1}{8}R[\tilde{D}]\right) + \psi^5\beta^i\tilde{D}_iK \tag{4.80}$$

Therefore, the system of elliptic equations to be solved for ψ, $\alpha\psi$ and β^i consists of (4.78), (4.80) and the Hamiltonian constraint (4.11) (with $\tilde{A}^{ij}$ set to be equal to the RHS of (4.77)).

Having written down the elliptic equations, it remains to specify suitable boundary conditions. Following [114], one can solve the system in a region with a single asymptotically flat end and a finite number of interior boundaries, corresponding to the apparent horizons of the black holes. The boundary conditions at spatial infinity are

$$\lim_{r\to\infty}\psi = 1, \qquad \lim_{r\to\infty}\alpha = 1, \qquad \lim_{r\to\infty}\beta^i = \Omega_{\rm orb}\epsilon^{ijk}e_jx_k \tag{4.81}$$

where $\Omega_{\rm orb}$ is the orbital angular velocity of the system, as measured at infinity and e^i is the unit vector specifying the axis of rotation. One may worry that with these boundary condition the shift vector diverges at spatial infinity. However, this is just an artefact of the corotating coordinates and the solution for β^i can be written as

$$\beta^i = \Omega_{\rm orb}\epsilon^{ijk}e_jx_k + \beta^i_{\rm reg}$$

where $\beta^i_{\rm reg}$ is regular and has the usual asymptotic fall-off. To make sure that the numerical evolution of this data is stable, one can simultaneously work in two different coordinate system [115]: one of them is the corotating coordinate system just described, the other one is "inertial".

To fix the boundary conditions on the interior boundaries, one can proceed as in [114] to require that the interior boundary surfaces correspond to apparent horizons. Let S be one of these 2-surfaces and let s^a be the unit normal (w.r.t. γ) to S. Then one can define the induced metric on S

$$P_{ij} = \gamma_{ij} - s_is_j \tag{4.82}$$

It is useful to introduce the conformally rescaled version of P_{ij} and s^i

$$P_{ij} = \psi^4\tilde{P}_{ij}, \qquad\qquad s_i = \psi^2\tilde{s}_i \tag{4.83}$$

Furthermore, let $\tilde{\mathcal{D}}$ denote the covariant derivative associated with $\tilde{P}$. Then one can impose the following requirements and a set of corresponding boundary conditions [114].

(1) First of all, one can construct a future-directed null vector field

$$k^\mu = \frac{1}{\sqrt{2}}(n^\mu + s^\mu)$$

and consider the null geodesic congruence with tangent vectors k^μ that pass through the surface S. These null geodesics determine a null hypersurface in the neighborhood of S. A possible notion of quasiequilibrium is to require that coordinate system initially tracks this null hypersurface, i.e. the coordinate location of the surface S does not change initially. Then this condition translates to $\left(\frac{\partial}{\partial t}\right)^\mu k_\mu\Big|_S = 0$ which implies

$$(\beta_\perp - \alpha)\Big|_S = 0, \qquad \beta^i_\perp \equiv \beta^i s_i \tag{4.84}$$

(2) The condition that the expansion of the null geodesic congruence defined above must be zero yields a Neumann-type boundary condition on the conformal factor

$$\left[\tilde{s}^k \tilde{D}_k \ln\psi - \frac{1}{4}\left(\psi^2 P^{ij} K_{ij} - \tilde{P}^{ij}\tilde{D}_i \tilde{s}_j\right)\right]\Bigg|_S = 0 \tag{4.85}$$

(3) The vanishing of the shear of the null geodesic congruence together with $\partial_t \tilde{\gamma}_{ij} = 0$ gives an equation for $\beta^i \equiv P^i{}_j \beta^j$

$$\left(\tilde{\mathcal{D}}^{(i}\beta^{j)}_\parallel - \frac{1}{2}\tilde{P}^{ij}\tilde{\mathcal{D}}_k \beta^k_\parallel\right)\Bigg|_S = 0. \tag{4.86}$$

Interestingly, this is just the conformal Killing equation on S. Since any closed 2d surface is conformally equivalent to the unit 2-sphere, the problem of solving (4.86) boils down to finding Killing vector fields on the unit 2-sphere. The unit 2-sphere has a family of rotational Killing vector fields ξ^i. Hence the vector

$$\beta^i_\parallel = \Omega_\mathrm{s}\xi^i \tag{4.87}$$

solves equation (4.86) for any constant parameter Ω_s. The parameter Ω_s determines the magnitude of the angular velocity of the black hole whereas ξ_i determines the axis of rotation.

(4) The boundary value of the lapse function α can be chosen freely as part of the initial temporal gauge freedom.

To summarize, the construction of initial data in quasiequilibrium amounts to solving the coupled system of elliptic equations (4.11), (4.78) and (4.80) subject to the boundary conditions (4.81), (4.84), (4.85), (4.87). The initial values of $\tilde{\gamma}_{ij}$, K are source terms in these equations and can be chosen freely, e.g. as $\tilde{\gamma}_{ij} = \delta_{ij}$ and $K = 0$ or as a "superposition" of two black hole solutions, see section 4.3.3.

4.4.2 The Conformal Thin Sandwich equations for scalar-tensor EFT

In this section we propose a way to adapt the extended CTS method for 4∂ST theories. For a scalar-tensor theory, we would like to derive elliptic equations for not only the variables ψ, α and β^i but also for the initial value of ϕ. Then the free part of the data consists of the initial values of $(\tilde{\gamma}, \partial_t\tilde{\gamma}, K, \partial_t K, K_\phi, \partial_t K_\phi)$.

The Hamiltonian and momentum constraints can be converted to elliptic equations in the exact same way as in GR: we can just take equations (4.47), (4.48) and substitute $\tilde{A}^{ij}$ with $\frac{\psi^6}{2\alpha}(\tilde{L}\beta)^{ij}$ (c.f. equation (4.77)) to impose quasiequilibrium.

To obtain the analogue of (4.80) and an elliptic equation for the scalar field, we start by considering the linear combination

$$\frac{1}{4}\alpha\psi^5\left(2\gamma^{\mu\nu}E_{\mu\nu} + \mathcal{H}\right) = 0$$

of the 4∂ST theory, write it in terms of the variables $\alpha, \beta, \tilde{\gamma}, \psi, K, \tilde{A}$ and impose a suitable quasiequilibrium condition. Introducing

$$\begin{aligned} \mathcal{A}_{kl} &= \frac{1}{\alpha}(\partial_t - \mathcal{L}_\beta)K_{kl} - K_{km}K^m{}_l - \frac{1}{\alpha}D_k D_l \alpha && (4.88)\\ \mathcal{A}_\phi &= \frac{1}{\alpha}(\partial_t - \mathcal{L}_\beta)K_\phi + \frac{1}{2\alpha}D^k\alpha D_k\phi && (4.89) \end{aligned}$$

and using the equations of Appendix 4.A, this combination yields

$$
\begin{aligned}
0 \;&=\; \tilde{\gamma}^{ij}\tilde{D}_i\tilde{D}_j(\alpha\psi) - \alpha\psi\left(\frac{7}{8}\psi^{-8}\tilde{A}_{ij}\tilde{A}^{ij} + \frac{5}{12}\psi^4K^2 + \frac{1}{8}R[\tilde{D}]\right) + \psi^5(\partial_t - \beta^i\tilde{D}_i)K \\
&\quad + \frac{1}{4}\alpha\psi^5\left\{\frac{5}{2}V(\phi) - 7K_\phi^2 + \frac{1}{4}\psi^{-4}\tilde{D}^i\phi\tilde{D}_i\phi + \delta E_{(\alpha\psi)}\right\}
\end{aligned} \tag{4.90}
$$

where

$$
\begin{aligned}
\delta E_{(\alpha\psi)} \;&\equiv\; 16\epsilon_2\gamma^{i[i_1}\gamma^{j]j_1}\left(D_{i_1}D_{j_1}f_2(\phi) - 2f_2'(\phi)K_\phi K_{i_1j_1}\right)\mathcal{A}_{ij} \\
&\quad -\frac{3}{4}\epsilon_1 f_1(\phi)XD^i\phi D_i\phi - 9\epsilon_1K_\phi^2 f_1(\phi)X \\
&\quad -\epsilon_2\gamma^{i_1i_2i_3}_{j_1j_2j_3}\left(R[D]_{i_1i_2}{}^{j_1j_2} + 2K_{i_1}{}^{j_1}K_{i_2}{}^{j_2}\right)\left(D_{i_3}D^{j_3}f_2(\phi) - 2f_2'(\phi)K_\phi K_{i_3}{}^{j_3}\right) \\
&\quad +4\epsilon_2\gamma^{i_1i_2}_{j_1j_2}\Bigg[2\left(\gamma^{j_3}_{i_1}\gamma^{j_1}_{i_3} + \gamma^{j_1j_3}\gamma_{i_1i_3}\right)\left(K_{j_3}{}^{k}D_kf_2(\phi) - 2D_{j_3}(f_2'(\phi)K_\phi)\right)D^{i_3}K_{i_2}{}^{j_2} \\
&\quad +\left(R[D]_{i_1i_2}{}^{j_1j_2} + 2K_{i_1}{}^{j_1}K_{i_2}{}^{j_2}\right)\left(f_2'(\phi)\mathcal{A}_\phi - 2f_2''(\phi)K_\phi^2\right)\Bigg]
\end{aligned} \tag{4.91}
$$

and the terms in $\delta E_{(\alpha\psi)}$ are to be converted to the conformal variables using the equations of Appendix 4.B. Equation (4.90) contains second time derivatives via the terms $\mathcal{A}_\phi$ and $\mathcal{A}_{ij}$. The natural way to impose quasiequilibrium on the data is to choose

$$
\partial_t\tilde{\gamma}_{ij} = 0, \qquad K_\phi = 0 \tag{4.92}
$$

and set the combination of time derivatives of K_{ij} and K_ϕ appearing in (4.90) to zero. Using these conditions in (4.90) and the scalar equation of motion yields an elliptic equation for the initial values of $\alpha\psi$ and ϕ:

$$
\begin{aligned}
0 \;&=\; \tilde{\gamma}^{ij}\tilde{D}_i\tilde{D}_j(\alpha\psi) - \alpha\psi\left(\frac{7}{8}\psi^{-8}\tilde{A}_{ij}\tilde{A}^{ij} + \frac{5}{12}\psi^4K^2 + \frac{1}{8}R[\tilde{D}]\right) - \psi^5\beta^i\tilde{D}_iK \\
&\quad \frac{1}{16}\alpha\psi^5\Big[(1 - 3\epsilon_1f_1(\phi)X)D^i\phi D_i\phi + 10\;V(\phi) + 4\delta E'_{(\alpha\psi)}\Big]
\end{aligned} \tag{4.93}
$$

$$
\begin{aligned}
0 \;&=\; (1 + 6\epsilon_1f_1(\phi)X)\left(\tilde{D}^k\tilde{D}_k\phi + 2\tilde{D}^k\phi\tilde{D}_k\ln\psi\right) \\
&\quad -\psi^4V'(\phi) + \tilde{D}^i\phi\tilde{D}_i\ln\alpha + \psi^4\delta E_{(\phi)}
\end{aligned} \tag{4.94}
$$

where

$$
\begin{aligned}
\delta E'_{(\alpha\psi)} \equiv & -16\epsilon_2\gamma^{i[i_1}\gamma^{j]j_1}D_{i_1}D_{j_1}f_2(\phi)\left(K_{ik}K^k{}_j+\frac{1}{\alpha}D_iD_j\alpha\right) \\
& -\epsilon_2\gamma^{i_1i_2i_3}_{j_1j_2j_3}\left(R[D]_{i_1i_2}{}^{j_1j_2}+2K_{i_1}{}^{j_1}K_{i_2}{}^{j_2}\right)D_{i_3}D^{j_3}f_2(\phi) \\
& +4\epsilon_2\gamma^{i_1i_2}_{j_1j_2}\Bigg[f_2'(\phi)\frac{1}{2\alpha}D^k\alpha D_k\phi\left(R[D]_{i_1i_2}{}^{j_1j_2}+2K_{i_1}{}^{j_1}K_{i_2}{}^{j_2}\right) \\
& \qquad +2\left(\gamma^{j_3}_{i_1}\gamma^{j_1}_{i_3}+\gamma^{j_1j_3}\gamma_{i_1i_3}\right)K_{j_3}{}^kD_kf_2(\phi)D^{i_3}K_{i_2}{}^{j_2}\Bigg] \\
\delta E_{(\phi)} \equiv & \ 2\epsilon_1f_1(\phi)\gamma^{i_1i_2}_{j_1j_2}D_{i_1}\phi D^{j_1}\phi D_{i_2}D^{j_2}\phi-\epsilon_1f_1(\phi)(D\phi)^2D^i\phi D_i\ln\alpha \\
& -\frac{3}{4}\epsilon_1f_1'(\phi)(D^k\phi D_k\phi)^2+8\epsilon_2f_2'(\phi)\gamma^{i_1i_2i_3}_{j_1j_2j_3}D^{j_1}K_{i_2}{}^{j_2}D_{i_1}K_{i_3}{}^{j_3} \\
& -2\epsilon_2f_2'(\phi)\gamma^{ii_1i_2}_{jj_1j_2}\left(R[D]_{i_1i_2}{}^{j_1j_2}+2K_{i_1}{}^{j_1}K_{i_2}{}^{j_2}\right)\left(\frac{1}{\alpha}D_iD^j\alpha+K_{ik}K^{jk}\right)
\end{aligned}
$$

Of course, again, these expressions need to be rewritten in terms of the conformal variables. Since this procedure is straightforward (using the identities of Appendix 4.B) but not particularly enlightening, we spare the reader from detailing these equations in their full lengths.

The final step in the construction is to impose boundary conditions. The apparent horizon and asymptotic boundary conditions on the gravitational variables can be taken to be the same as in section 4.4.1 (equations (4.81), (4.84), (4.85), (4.87)). Regarding the scalar field, it is simplest to choose

$$
\lim_{r\to\infty}\phi=\phi_\infty \qquad \text{and} \qquad s^i\partial_i\phi\Big|_S=0 \tag{4.95}
$$

where s^i is the unit normal to the interior boundary S and ϕ_∞ is a constant. For a single stationary black hole, the latter condition captures the property that there is no scalar flux through the horizon.

To conclude our proposal, the extended conformal thin sandwich method for the scalar-tensor theory (1.5) amounts to solving the elliptic equations (4.47), (4.48), (4.93) and (4.94) for the variables $(\psi, \beta^i, \alpha, \phi)$ subject to the boundary conditions (4.81), (4.84), (4.85), (4.87) and (4.95). The (remaining) free part of the data $(\tilde{\gamma}, K)$ can be fixed using the methods of section 4.3.3.

4.4.3 On the existence and uniqueness of the extended Conformal Thin Sandwich system

The problem of existence and uniqueness of the extended conformal thin sandwich system is more complicated than in the case of the CTT or the original CTS system, even in general relativity. In particular, the issue is with the extra equation (4.80). Concentrate on the terms in (4.80)

$$\tilde{\gamma}^{ij}\tilde{D}_i\tilde{D}_j(\alpha\psi) - \alpha\psi\left(\frac{7}{8}\psi^{-8}\tilde{A}_{ij}\tilde{A}^{ij}\right) = \tilde{\gamma}^{ij}\tilde{D}_i\tilde{D}_j(\alpha\psi) - \frac{7}{32}\psi^{6}(\tilde{L}\beta)^{ij}(\tilde{L}\beta)_{ij}(\alpha\psi)^{-1}$$

Upon linearization of (4.80), this part of the equation gives rise to the terms

$$\tilde{\gamma}^{ij}\tilde{D}_i\tilde{D}_j\delta(\alpha\psi) + \frac{7}{32}(\alpha\psi)^{-2}\psi^{6}(\tilde{L}\beta)^{ij}(\tilde{L}\beta)_{ij}\delta(\alpha\psi) + ... = 0$$

However, for a linear elliptic equation of the form

$$\tilde{\gamma}^{ij}\tilde{D}_i\tilde{D}_j\Phi - c\Phi = 0$$

with a function c, the uniqueness of the solution may fail if c is negative[4]. Therefore, one could find solutions so that $(\tilde{L}\beta)^{ij}(\tilde{L}\beta)_{ij}$ is large enough and the linearized version of (4.80) does not have a unique solution.

Going beyond this toy argument, it has been explicitly demonstrated [102, 116–118] (both numerically and by means of bifurcation theory) that there exists choices of free data for the extended CTS system such that the corresponding solution is not unique. Nevertheless, the extended CTS approach has been used in several numerical simulations to construct binary black hole initial data (see e.g. [84] and the references therein).

Similar issues may be expected in the scalar-tensor version of the extended CTS method. In addition to this, the scalar elliptic equation (4.94) may also suffer from this type of failure of uniqeness under some choice of the potential $V(\phi)$ and the couplings $f_1(\phi)$, $f_2(\phi)$. In fact, there is already some numerical evidence that this may happen. Several recent studies focused on stationary, axisymmetric black hole solutions of the theory $f_1(\phi) = V(\phi) = 0$, $f_2(\phi) = \eta\phi^2$ where η is a constant (see e.g. [28, 29, 119–121]). These studies concluded that if the coupling constant η is large enough (i.e. in the strongly coupled regime where η has order of magnitude M^2 where M is the mass of the black

[4] The solution is unique on asymptotically Euclidean manifolds when $c \geq 0$, c.f. Lemma 4.2.

hole) then the Kerr spacetime is no longer the unique rotating black hole solution: for fixed mass and angular momentum, there exists another solution with a nontrivial scalar configuration. Moreover, the scalarized solution appears to be stable. More generally, $\phi = 0$ is a solution to $E_\phi = 0$ and the theory inherits solutions of vacuum general relativity. Consider the simple case when the initial slice has a single interior boundary and the free data $(\tilde{\gamma}, K)$ is chosen to be the induced metric and the trace of the extrinsic curvature of a slice of the Kerr spacetime (e.g. a Kerr-Schild slice). Clearly, for this particular theory, $\phi = 0$ is a solution to (4.94) (provided that $\phi_\infty = 0$). Then the extended CTS equations are the same as in vacuum GR and they reproduce a slice of the Kerr solution [98]. However, for large enough η, (4.94) is likely to have a bifurcating branch of solutions: for a choice of free data that represents a slice of a Kerr black hole, there will be a solution with a non-trivial scalar field configuration in addition to the solution with $\phi \equiv 0$. There is no reason to expect that the solution with non-trivial ϕ is an exact slice of the stationary scalar hairy black hole solution found in [28, 29, 119–121]. Instead, this data is more likely to represent a slice of a dynamical black hole that may eventually settle down to the stationary scalar hairy black hole of [28, 29, 119–121] when evolved in time. To obtain data that is a more accurate representation of a slice of a scalarized stationary black hole, one could choose the free data $(\tilde{\gamma}, K)$ to be the induced metric and the trace of the extrinsic curvature of a constant time slice of the scalarized black hole solution. The construction of initial data for a binary system of such black holes could then be done by using the idea of "superposition" (section 4.3.3) to choose the free data.

Appendix 4.A Evolution equations of scalar-tensor effective theories in a $3 + 1$ form

In this appendix we provide the evolution equations of the 4∂ST theories written in terms of the ADM variables. These equations can be found in e.g. [110] for the theories with $f_1(\phi) \equiv 0$. The main reason for giving these equations is that our convention for the scalar field is slightly different from that of [110].

Following [110], it is useful to introduce

$$\mathcal{A}_{kl} = \frac{1}{\alpha}(\partial_t - \mathcal{L}_\beta)K_{kl} - K_{km}K^m{}_l - \frac{1}{\alpha}D_k D_l \alpha \tag{4.96}$$

$$\mathcal{A}_\phi = \frac{1}{\alpha}(\partial_t - \mathcal{L}_\beta)K_\phi + \frac{1}{2\alpha}D^k \alpha D_k \phi \tag{4.97}$$

The evolution equations of 4∂ST theories are the spatial components of the gravitational equation of motion and the scalar equation of motion. These can be written as

$$E_{ij} \equiv \frac{\partial(\gamma^{-1/2}\pi_{ij})}{\partial K_{kl}}\mathcal{A}_{kl} + \frac{\partial(\gamma^{-1/2}\pi_{ij})}{\partial K_{\phi}}\mathcal{A}_{\phi} - \mathcal{F}_{ij} = 0 \tag{4.98}$$

$$E_{\phi} \equiv \frac{\partial(\gamma^{-1/2}\pi_{\phi})}{\partial K_{kl}}\mathcal{A}_{kl} + \frac{\partial(\gamma^{-1/2}\pi_{\phi})}{\partial K_{\phi}}\mathcal{A}_{\phi} - \mathcal{F}_{\phi} = 0 \tag{4.99}$$

with

$$\begin{aligned}
\mathcal{F}^{i}{}_{j} = & -\frac{1}{2}(1+2\epsilon_1 f_1(\phi)X)D^i\phi D_j\phi + \frac{1}{2}V(\phi)\gamma^i_j \\
& +\frac{1}{4}\gamma^i_j\left(D^k\phi D_k\phi - 4K_\phi^2\right)(1+\epsilon_1 f_1(\phi)X) \\
& -\frac{1}{4}\gamma^{ii_1i_2}_{jj_1j_2}\Big[16\epsilon_2\left(\gamma^{j_3}_{i_1}\gamma^{j_1}_{i_3} + \gamma^{j_1j_3}\gamma_{i_1i_3}\right)\left(-K_{j_3}{}^k D_k f_2(\phi) + 2D_{j_3}(f_2'(\phi)K_\phi)\right)D^{i_3}K_{i_2}{}^{j_2} \\
& + \left(R[D]_{i_1i_2}{}^{j_1j_2} + 2K_{i_1}{}^{j_1}K_{i_2}{}^{j_2}\right)\left(1+16\epsilon_2 f_2''(\phi)K_\phi^2\right)\Big]
\end{aligned} \tag{4.100}$$

$$\begin{aligned}
\mathcal{F}_{\phi} = & -V'(\phi) + (1+6\epsilon_1 f_1(\phi)X - 8\epsilon_1 f_1(\phi)K_\phi^2)\left(D^kD_k\phi - 2KK_\phi\right) \\
& -3\epsilon_1 f_1'(\phi)X^2 - 8\epsilon_1 f_1(\phi)K_\phi\left(K_i{}^jD_j\phi D^i\phi - 2D_iK_\phi D^i\phi\right) \\
& +2\epsilon_1 f_1(\phi)\gamma^{i_1i_2}_{j_1j_2}D_{i_1}\phi D^{j_1}\phi\left(D_{i_2}D^{j_2}\phi - 2K_\phi K_{i_2}{}^{j_2}\right) \\
& +8\epsilon_2 f_2'(\phi)\gamma^{i_1i_2i_3}_{j_1j_2j_3}D^{j_1}K_{i_2}{}^{j_2}D_{i_1}K_{i_3}{}^{j_3}
\end{aligned} \tag{4.101}$$

and the coefficients of the time derivatives are

$$\frac{\partial(\gamma^{-1/2}\pi^i{}_j)}{\partial K^k{}_l} = \gamma^{il}_{jk} - 4\epsilon_2\gamma^{ili_1}_{jkj_1}\left(D_{i_1}D^{j_1}f_2(\phi) - 2f_2'(\phi)K_\phi K_{i_1}{}^{j_1}\right) \tag{4.102}$$

$$\begin{aligned}
\frac{\partial(\gamma^{-1/2}\pi^i{}_j)}{\partial K_\phi} &= \frac{\partial(\gamma^{-1/2}\pi_\phi)}{\partial K_i{}^j} \\
&= -2\epsilon_2 f_2'(\phi)\gamma^{ii_1i_2}_{jj_1j_2}\left(R[D]_{i_1i_2}{}^{j_1j_2} + 2K_{i_1}{}^{j_1}K_{i_2}{}^{j_2}\right)
\end{aligned} \tag{4.103}$$

$$\frac{\partial(\gamma^{-1/2}\pi_\phi)}{\partial K_\phi} = -2\left(1+6\epsilon_1 f_1(\phi)X + 2\epsilon_1 f_1(\phi)(D\phi)^2\right) \tag{4.104}$$

Appendix 4.B Conformal decomposition

In this section, we collected some identities for converting the elliptic equations to their conformal form. First of all, we have

$$X \equiv -\frac{1}{2}(\nabla\phi)^2 = 2\psi^{-12}\tilde{K}_\phi^2 - \frac{1}{2}\psi^{-4}\tilde{\gamma}^{ij}\tilde{D}_i\phi\tilde{D}_j\phi \tag{4.105}$$

For a general scalar function Φ, we have

$$D_i D^j \Phi = \psi^{-4}\tilde{D}_i\tilde{D}^j\Phi - 2\psi^{-4}\tilde{D}_k\Phi\left(\gamma_i^k\tilde{D}^j\ln\psi + \tilde{\gamma}^{jk}\tilde{D}_i\ln\psi - \gamma_i^j\tilde{\gamma}^{kl}\tilde{D}_l\ln\psi\right) \tag{4.106}$$

and in particular,

$$D_i D^i \Phi = \psi^{-4}\left(\tilde{\gamma}^{ij}\tilde{D}_i\tilde{D}_j\Phi + 2\tilde{\gamma}^{ij}\tilde{D}_i\ln\psi\tilde{D}_j\Phi\right) \tag{4.107}$$

The conformal transformation rule for the Riemann tensor is

$$\begin{aligned} R[D]_{i_1 i_2}{}^{j_1 j_2} &= \psi^{-4}R[\tilde{D}]_{i_1 i_2}{}^{j_1 j_2} - 8\psi^{-5}\gamma^{[j_1}_{[i_1}\tilde{D}_{i_2]}\tilde{D}^{j_2]}\psi \\ &\quad +24\psi^{-6}\gamma^{[j_1}_{[i_1}\tilde{D}_{i_2]}\psi\tilde{D}^{j_2]}\psi - 4\gamma^{j_1 j_2}_{i_1 i_2}\psi^{-6}\tilde{\gamma}^{kl}\tilde{D}_k\psi\tilde{D}_l\psi \end{aligned} \tag{4.108}$$

To convert products of the extrinsic curvature to conformal variables, the following may be useful:

$$\begin{aligned} \gamma^{i_1 i_2 i_3}_{j_1 j_2 j_3}K_{i_1}{}^{j_1}K_{i_2}{}^{j_2} &= \frac{2}{9}K^2\gamma^{i_3}_{j_3} - \frac{2}{3}\psi^{-6}K\tilde{A}^{i_3}_{j_3} \\ &\quad +2\psi^{-12}\tilde{A}^{i_3}{}_k\tilde{A}^k{}_{j_3} - \psi^{-12}\tilde{A}^k{}_l\tilde{A}^l{}_k\gamma^{i_3}_{j_3} \end{aligned} \tag{4.109}$$

Finally, for the derivatives of the extrinsic curvature, one can use

$$\begin{aligned} D^j K_{i_1}{}^{j_1} &= \psi^{-10}\tilde{D}^j\tilde{A}_{i_1}{}^{j_1} + \frac{1}{3}\psi^{-4}\tilde{\gamma}_{i_1}{}^{j_1}\tilde{D}^j K - 6\psi^{-10}\tilde{A}_{i_1}{}^{j_1}\tilde{D}^j\ln\psi \\ &\quad +2\psi^{-10}\Big(\tilde{\gamma}^{jj_1}\tilde{A}_{i_1}{}^l\tilde{D}_l\ln\psi + \tilde{\gamma}_{i_1}{}^j\tilde{A}^{j_1 l}\tilde{D}_l\ln\psi \\ &\quad -\tilde{A}_{i_1}{}^j\tilde{D}^{j_1}\ln\psi - \tilde{A}^{jj_1}\tilde{D}_{i_1}\ln\psi\Big) \end{aligned} \tag{4.110}$$

Chapter 5

Conclusions

This thesis explored some mathematical properties of two classes of effective theories of gravity with second order equations of motion: Lovelock and Horndeski theories. These theories attracted considerable research interest in recent times due to their possible relevance to cosmology and high energy physics.

The majority of the thesis focuses on the initial value problem in Lovelock and Horndeski theories. The main result presented here is that these two theories possess a locally well-posed initial value formulation when the theories are weakly coupled. Weak coupling means that the Lovelock or Horndeski corrections are small compared to the Einstein-scalar-field theory terms in the equations of motion. The remainder of the thesis addresses the initial data problem for 4-derivative scalar-tensor effective field theories (a class of Horndeski theories). It was shown that the constraint equations of the theory have solutions on asymptotically flat initial data surfaces. These results demonstrate that Lovelock and Horndeski theories satisfy some important mathematical consistency requirements, at least for small couplings.

To gain some insight into the initial value problem for general Lovelock and Horndeski theories, it was useful to study cubic Horndeski theories in detail. In chapter 2 we have provided three locally well-posed formulations of this class of theories at weak coupling. The proofs of these results relied on a special property of the cubic Horndeski equations of motion: terms containing the spacetime curvature in the scalar equation of motion can be eliminated using the gravitational equation of motion. We have exploited this property to derive an alternative scalar equation of motion which greatly simplified the analysis of well-posedness.

The first two well-posed formulations presented in chapter 2 are generalizations of the BSSN and the CCZ4 systems. The BSSN-type and CCZ4-type formulations of weakly coupled cubic Horndeski theories are found to be strongly hyperbolic when the free functions describing the slicing and shift conditions obey suitable bounds. These bounds are enforced by the criterion that the causal cone associated with the scalar degree of freedom must not intersect the causal cones associated with certain "non-physical" degrees of freedom. Violation of this condition leads to a failure of strong hyperbolicity of the equations of motion.

The third well-posed formulation of cubic Horndeski theories discussed in chapter 2 is an extension of an elliptic-hyperbolic formulation of general relativity. The gauge-fixed equations are obtained using the spatial harmonic gauge condition and a generalization of the constant mean curvature slicing condition. The elliptic equations are modifications of the cubic Horndeski constraint equations. These elliptic constraint equations can be uniquely solved for the lapse function and the shift vector on compact spatial slices with negative Ricci curvature. When the elliptic constraints hold, and the cubic Horndeski couplings are sufficiently small, the evolution equations are strongly hyperbolic.

Despite the success of these three methods for cubic Horndeski theories, it appears that they do not lead to a well-posed formulation of more general Horndeski or Lovelock theories. One of the reasons for this failure is that the equations of motion of more complicated Horndeski theories do not have the same special structure as the equations of cubic Horndeski theories: there seems to be no obvious way to simplify the scalar equation of motion by modifying it with a linear combination of the gravitational equations of motion. The second problem is the degeneracy between certain mode solutions of the equations. An appropriate choice of the gauge source functions in the BSSN and CCZ4 formulations removes the degeneracy between some but not all of the "unphysical" modes. The remaining degeneracy between pure gauge and constraint violating modes typically leads to a failure of strong hyperbolicity in a general Horndeski or Lovelock theory, even at small couplings.

One solution to this problem is given in chapter 3 where we introduce a modified harmonic gauge condition and gauge-fixing of the gravitational equations of motion of the theories discussed. This approach involves two auxiliary Lorentzian metrics: one of them specifies the gauge condition, and the other determines how the gauge condition modifies the equations. The degeneracy between different types of high-frequency mode solutions is resolved when the causal cones of the two auxiliary metrics and the spacetime metric form a nested set (see Fig. 3.1). Further investigation of the modified harmonic equations in general relativity reveals that this simple condition on the causal cones is sufficient for strong hyperbolicity. A continuity argument establishes that the modified harmonic gauge Lovelock and Horndeski equations are also strongly hyperbolic at sufficiently small couplings.

An important mathematical problem related to the Cauchy problem concerns the construction of initial data in gravitational theories. Clearly, this is an essential starting point to study the dynamics of the theories. The problem is to find solutions to the gravitational constraint equations that represent a sufficiently broad class of astrophysical objects.

In chapter 4, we considered the initial data problem on asymptotically Euclidean hypersurfaces in a class of (weakly coupled) scalar-tensor effective theories, using standard conformal techniques of general relativity and results from the elliptic PDE literature. These methods seem to be quite robust and are applicable in more general settings. For example, we did not make use of the specific form of the equations of motion, so it seems likely that the construction of asymptotically Euclidean initial data works similarly for any weakly coupled Horndeski or even Lovelock theories.

The results presented in chapter 4 for the CTT and CTS systems have the obvious possible application to construct black hole binary initial data numerically that could be evolved using the modified harmonic formulation. The puncture data (which is based on the CTT approach) has the advantage that it only requires solving a single elliptic equation (the Hamiltonian constraint) coupled to a set of algebraic equations. The main drawback of this method (besides the presence of junk radiation in the data and the possible need for excision) is that there appears to be no simple and natural candidate for the scalar field initial data. In the conformal thin sandwich method, one needs to solve a coupled system of elliptic equations for the conformal factor and the shift vector, which may be computationally more costly than the puncture method. However, if the 4-derivative EFT couplings are sufficiently weak, these equations may be solved iteratively, starting from GR initial data. Furthermore, the free part of the data may be fixed using standard methods of numerical relativity, e.g. by "superposing" stationary scalar hairy black hole solutions.

Overall, this thesis demonstrated the importance of studying the mathematical properties of Horndeski and Lovelock theories. We also provided solutions to the local Cauchy problem and the initial data problem in these theories, which may also be relevant for numerical relativity and observational tests of general relativity. The results presented here open up the possibility to explore other interesting problems related to these (and possibly other) effective theories of gravity.

For example, one may be interested in whether the weakly coupled assumption could be violated dynamically. The nonlinear evolution of the equations could drive the fields out of the regime where the Horndeski or Lovelock terms are small compared to the Einstein-scalar-field theory terms, even if one starts with weakly coupled initial data. This is certainly a real concern since the results presented in this paper only guarantee *local* well-posedness. The long time behaviour of the system, however, is a question of *global* well-posedness, which is a very subtle and complicated problem to solve rigorously even in general relativity. Nonetheless, there are some recent numerical studies on some Horndeski theories indicating that the formulations presented here may give rise to global solutions under certain conditions [66, 70].

Of course, it is also possible that the modified harmonic gauge Horndeski equations of motion are strongly hyperbolic even at *strong couplings* for a sufficiently broad class of field configurations (at least for some choice of the coupling functions). In particular, it is likely to be the case in theories whose gauge invariant characteristic polynomial (introduced in [45]) is a hyperbolic polynomial in a generic class of strongly coupled solutions. It would be interesting to see if there are theories and a class of solutions satisfying this condition.

Finally, another application of the ideas explored in this thesis could be to investigate the causal structure of weakly coupled effective theories of gravity in more detail [45].

References

[1] A. Einstein, Die Feldgleichungen der Gravitation, Sitzungsberichte der Königlich Preußischen Akademie der Wissenschaften (Berlin (1915) 844–847.

[2] C. M. Will, The Confrontation between General Relativity and Experiment, Living Rev. Rel. 17 (2014) 4. doi:10.12942/lrr-2014-4.

[3] F. W. Dyson, A. S. Eddington, C. Davidson, A Determination of the Deflection of Light by the Sun's Gravitational Field, from Observations Made at the Total Eclipse of May 29, 1919, Philosophical Transactions of the Royal Society of London Series A 220 (1920) 291–333. doi:10.1098/rsta.1920.0009.

[4] R. Penrose, Gravitational collapse and space-time singularities, Phys. Rev. Lett. 14 (1965) 57–59. doi:10.1103/PhysRevLett.14.57.

[5] R. Penrose, Gravitational collapse: The role of general relativity, Riv. Nuovo Cim. 1 (1969) 252–276. doi:10.1023/A:1016578408204.

[6] A. M. Ghez, B. L. Klein, M. Morris, E. E. Becklin, High proper-motion stars in the vicinity of sagittarius $a*$: Evidence for a supermassive black hole at the center of our galaxy, The Astrophysical Journal 509 (2) (1998) 678–686. doi:10.1086/306528.

[7] S. Gillessen, F. Eisenhauer, S. Trippe, T. Alexander, R. Genzel, F. Martins, T. Ott, Monitoring stellar orbits around the Massive Black Hole in the Galactic Center, Astrophys. J. 692 (2009) 1075–1109. doi:10.1088/0004-637X/692/2/1075.

[8] K. Akiyama, et al., First M87 Event Horizon Telescope Results. I. The Shadow of the Supermassive Black Hole, Astrophys. J. Lett. 875 (2019) L1. doi:10.3847/2041-8213/ab0ec7.

[9] B. P. Abbott, et al., Observation of Gravitational Waves from a Binary Black Hole Merger, Phys. Rev. Lett. 116 (6) (2016) 061102. doi:10.1103/PhysRevLett.116.061102.

[10] S. W. Hawking, R. Penrose, The Singularities of gravitational collapse and cosmology, Proc. Roy. Soc. Lond. A 314 (1970) 529–548. doi:10.1098/rspa.1970.0021.

[11] S. Endlich, V. Gorbenko, J. Huang, L. Senatore, An effective formalism for testing extensions to general relativity with gravitational waves, JHEP 09 (2017) 122. doi:10.1007/JHEP09(2017)122.

[12] E. E. Flanagan, R. M. Wald, Does back reaction enforce the averaged null energy condition in semiclassical gravity?, Phys. Rev. D54 (1996) 6233–6283. doi:10.1103/PhysRevD.54.6233.

[13] C. P. Burgess, Quantum gravity in everyday life: General relativity as an effective field theory, Living Rev. Rel. 7 (2004) 5–56. doi:10.12942/lrr-2004-5.

[14] M. Ostrogradsky, Mémoires sur les équations différentielles, relatives au problème des isopérimètres, Mem. Acad. St. Petersbourg 6 (4) (1850) 385–517.

[15] R. P. Woodard, Avoiding dark energy with 1/r modifications of gravity, Lect. Notes Phys. 720 (2007) 403–433. doi:10.1007/978-3-540-71013-4_14.

[16] L. Parker, J. Z. Simon, Einstein equation with quantum corrections reduced to second order, Phys. Rev. D 47 (1993) 1339–1355. arXiv:gr-qc/9211002, doi:10.1103/PhysRevD.47.1339.

[17] W. Israel, J. M. Stewart, Transient relativistic thermodynamics and kinetic theory, Annals Phys. 118 (1979) 341–372. doi:10.1016/0003-4916(79)90130-1.

[18] A. R. Solomon, M. Trodden, Higher-derivative operators and effective field theory for general scalar-tensor theories, JCAP 02 (2018) 031. arXiv:1709.09695, doi:10.1088/1475-7516/2018/02/031.

[19] G. Allwright, L. Lehner, Towards the nonlinear regime in extensions to GR: assessing possible options, Class. Quant. Grav. 36 (8) (2019) 084001. doi:10.1088/1361-6382/ab0ee1.

[20] R. P. Geroch, Relativistic theories of dissipative fluids, J. Math. Phys. 36 (1995) 4226. doi:10.1063/1.530958.

[21] H. S. Reall, C. M. Warnick, Effective field theory and classical equations of motion (5 2021). arXiv:2105.12028.

[22] S. Weinberg, Effective Field Theory for Inflation, Phys. Rev. D77 (2008) 123541. doi:10.1103/PhysRevD.77.123541.

[23] P. Kanti, N. E. Mavromatos, J. Rizos, K. Tamvakis, E. Winstanley, Dilatonic black holes in higher curvature string gravity, Phys. Rev. D 54 (1996) 5049–5058. doi:10.1103/PhysRevD.54.5049.

[24] B. Kleihaus, J. Kunz, E. Radu, Rotating Black Holes in Dilatonic Einstein-Gauss-Bonnet Theory, Phys. Rev. Lett. 106 (2011) 151104. doi:10.1103/PhysRevLett.106.151104.

[25] B. Kleihaus, J. Kunz, S. Mojica, E. Radu, Spinning black holes in Einstein–Gauss-Bonnet–dilaton theory: Nonperturbative solutions, Phys. Rev. D 93 (4) (2016) 044047. doi:10.1103/PhysRevD.93.044047.

[26] T. P. Sotiriou, S.-Y. Zhou, Black hole hair in generalized scalar-tensor gravity: An explicit example, Phys. Rev. D 90 (2014) 124063. doi:10.1103/PhysRevD.90.124063.

[27] J. F. M. Delgado, C. A. R. Herdeiro, E. Radu, Spinning black holes in shift-symmetric Horndeski theory, JHEP 04 (2020) 180. doi:10.1007/JHEP04(2020)180.

[28] D. D. Doneva, S. S. Yazadjiev, New Gauss-Bonnet Black Holes with Curvature-Induced Scalarization in Extended Scalar-Tensor Theories, Phys. Rev. Lett. 120 (13) (2018) 131103. doi:10.1103/PhysRevLett.120.131103.

[29] P. V. P. Cunha, C. A. R. Herdeiro, E. Radu, Spontaneously Scalarized Kerr Black Holes in Extended Scalar-Tensor–Gauss-Bonnet Gravity, Phys. Rev. Lett. 123 (1) (2019) 011101. doi:10.1103/PhysRevLett.123.011101.

[30] B. Zwiebach, Curvature Squared Terms and String Theories, Phys. Lett. B 156 (1985) 315–317. doi:10.1016/0370-2693(85)91616-8.

[31] R. R. Metsaev, A. A. Tseytlin, Order alpha-prime (Two Loop) Equivalence of the String Equations of Motion and the Sigma Model Weyl Invariance Conditions: Dependence on the Dilaton and the Antisymmetric Tensor, Nucl. Phys. B 293 (1987) 385–419. doi:10.1016/0550-3213(87)90077-0.

[32] D. Lovelock, The Einstein Tensor and Its Generalizations, J. Math. Phys. 12 (1971) 498–501. doi:10.1063/1.1665613.

[33] C. Lanczos, Elektromagnetismus als natürliche Eigenschaft der Riemannschen Geometrie, Zeitschrift fur Physik 73 (3-4) (1932) 147–168. doi:10.1007/BF01351210.

[34] C. Lanczos, A Remarkable property of the Riemann-Christoffel tensor in four dimensions, Annals Math. 39 (1938) 842–850. doi:10.2307/1968467.

[35] G. W. Horndeski, Second-order scalar-tensor field equations in a four-dimensional space, Int. J. Theor. Phys. 10 (1974) 363–384. doi:10.1007/BF01807638.

[36] T. Kobayashi, M. Yamaguchi, J. Yokoyama, Generalized G-inflation: Inflation with the most general second-order field equations, Prog. Theor. Phys. 126 (2011) 511–529. doi:10.1143/PTP.126.511.

[37] L. C. Evans, Partial differential equations / Lawrence C. Evans (Department of Mathematics, University of California, Berkeley)., second edition. Edition, Graduate studies in mathematics ; v. 19, 2010.

[38] R. M. Wald, General Relativity, Chicago Univ. Pr., Chicago, USA, 1984. doi:10.7208/chicago/9780226870373.001.0001.

[39] G. Papallo, Causality and the initial value problem in Modified Gravity, Ph.D. thesis, Cambridge U., DAMTP (3 2018). doi:10.17863/CAM.24726.

[40] H.-O. Kreiss, J. Lorenz, Initial-boundary value problems and the Navier-Stokes equations, Vol. 136, Society for Industrial and Applied Mathematics, 1989. doi:10.1137/1.9780898719130.

[41] M. E. Taylor, Pseudodifferential Operators and Nonlinear PDE, Birkhäuser, Boston, MA, Boston, 1991. doi:10.1007/978-1-4612-0431-2.

[42] O. Sarbach, M. Tiglio, Continuum and Discrete Initial-Boundary Value Problems and Einstein's Field Equations, Living Rev. Relativ. 15 (2012) 191. `doi:10.12942/lrr-2012-9`.

[43] O. Sarbach, M. Tiglio, Exploiting gauge and constraint freedom in hyperbolic formulations of Einstein's equations, Phys. Rev. D 66 (2002) 064023. `doi:10.1103/PhysRevD.66.064023`.

[44] Á. D. Kovács, H. S. Reall, Well-posed formulation of Lovelock and Horndeski theories, Phys. Rev. D 101 (12) (2020) 124003. `doi:10.1103/PhysRevD.101.124003`.

[45] H. S. Reall, Causality in gravitational theories with second order equations of motion, Phys. Rev. D 103 (8) (2021) 084027. `doi:10.1103/PhysRevD.103.084027`.

[46] F. John, Blow-up for quasi-linear wave equations in three space dimensions, Communications on Pure and Applied Mathematics 34 (1) (1981) 29–51. `doi:https://doi.org/10.1002/cpa.3160340103`.

[47] D. Christodoulou, S. Klainerman, The Global nonlinear stability of the Minkowski space (1993).

[48] H. Lindblad, I. Rodnianski, Global existence for the Einstein vacuum equations in wave coordinates, Commun. Math. Phys. 256 (2005) 43–110. `doi:10.1007/s00220-004-1281-6`.

[49] Y. Choquet-Bruhat, Théorème d'existence pour certains systèmes d'équations aux dérivées partielles non linéaires, Acta Math. 88 (1952) 141–225.

[50] Y. Choquet-Bruhat, R. P. Geroch, Global aspects of the Cauchy problem in general relativity, Commun. Math. Phys. 14 (1969) 329–335. `doi:10.1007/BF01645389`.

[51] J. Sbierski, On the Existence of a Maximal Cauchy Development for the Einstein Equations - a Dezornification, Annales Henri Poincare 17 (2) (2016) 301–329. `doi:10.1007/s00023-015-0401-5`.

[52] H. Friedrich, On the hyperbolicity of einstein's and other gauge field equations, Communications in Mathematical Physics 100 (4) (1985) 525–543.

[53] M. Salgado, The Cauchy problem of scalar tensor theories of gravity, Class. Quant. Grav. 23 (2006) 4719–4742. `doi:10.1088/0264-9381/23/14/010`.

[54] A. D. Rendall, Dynamics of k-essence, Class. Quant. Grav. 23 (2006) 1557–1570. `doi:10.1088/0264-9381/23/5/008`.

[55] O. Sarbach, E. Barausse, J. A. Preciado-López, Well-posed Cauchy formulation for Einstein-æther theory, Class. Quant. Grav. 36 (16) (2019) 165007. `doi:10.1088/1361-6382/ab2e13`.

[56] T. Delsate, D. Hilditch, H. Witek, Initial value formulation of dynamical Chern-Simons gravity, Phys. Rev. D 91 (2) (2015) 024027. `doi:10.1103/PhysRevD.91.024027`.

[57] H. Witek, L. Gualtieri, P. Pani, T. P. Sotiriou, Black holes and binary mergers in scalar Gauss-Bonnet gravity: scalar field dynamics, Phys. Rev. D99 (6) (2019) 064035. doi:10.1103/PhysRevD.99.064035.

[58] M. Okounkova, L. C. Stein, M. A. Scheel, D. A. Hemberger, Numerical binary black hole mergers in dynamical Chern-Simons gravity: Scalar field, Phys. Rev. D 96 (4) (2017) 044020. doi:10.1103/PhysRevD.96.044020.

[59] H. S. Reall, N. Tanahashi, B. Way, Causality and hyperbolicity of Lovelock theories, Class. Quantum Gravity 31 (2014) 205005. doi:10.1088/0264-9381/31/20/205005.

[60] G. Papallo, H. S. Reall, On the local well-posedness of Lovelock and Horndeski theories, Phys. Rev. D96 (4) (2017) 044019. doi:10.1103/PhysRevD.96.044019.

[61] G. Papallo, On the hyperbolicity of the most general Horndeski theory, Phys. Rev. D96 (12) (2017) 124036. doi:10.1103/PhysRevD.96.124036.

[62] J. L. Ripley, F. Pretorius, Hyperbolicity in Spherical Gravitational Collapse in a Horndeski Theory, Phys. Rev. D99 (8) (2019) 084014. doi:10.1103/PhysRevD.99.084014.

[63] J. L. Ripley, F. Pretorius, Gravitational collapse in Einstein dilaton-Gauss–Bonnet gravity, Class. Quant. Grav. 36 (13) (2019) 134001. doi:10.1088/1361-6382/ab2416.

[64] J. L. Ripley, F. Pretorius, Scalarized Black Hole dynamics in Einstein dilaton Gauss-Bonnet Gravity, Phys. Rev. D101 (4) (2020) 044015. doi:10.1103/PhysRevD.101.044015.

[65] L. Bernard, L. Lehner, R. Luna, Challenges to global solutions in Horndeski's theory, Phys. Rev. D 100 (2) (2019) 024011. doi:10.1103/PhysRevD.100.024011.

[66] P. Figueras, T. França, Gravitational Collapse in Cubic Horndeski Theories, Class. Quant. Grav. 37 (22) (2020) 225009. doi:10.1088/1361-6382/abb693.

[67] A. D. Kovács, Well-posedness of cubic Horndeski theories, Phys. Rev. D100 (2) (2019) 024005. doi:10.1103/PhysRevD.100.024005.

[68] Á. D. Kovács, H. S. Reall, Well-posed formulation of scalar-tensor effective field theory, Phys. Rev. Lett. 124 (22) (2020) 221101. doi:10.1103/PhysRevLett.124.221101.

[69] M. Okounkova, Numerical relativity simulation of GW150914 in Einstein dilaton Gauss-Bonnet gravity, Phys. Rev. D 102 (8) (2020) 084046. doi:10.1103/PhysRevD.102.084046.

[70] W. E. East, J. L. Ripley, Evolution of Einstein-scalar-Gauss-Bonnet gravity using a modified harmonic formulation, Phys. Rev. D 103 (4) (2021) 044040. doi:10.1103/PhysRevD.103.044040.

[71] A. De Felice, S. Tsujikawa, Cosmology of a Covariant Galileon Field, Phys. Rev. Lett. 105 (2010) 111301. doi:10.1103/PhysRevLett.105.111301.

[72] A. De Felice, S. Tsujikawa, Generalized Galileon cosmology, Phys. Rev. D 84 (2011) 124029. doi:10.1103/PhysRevD.84.124029.

[73] T. Kobayashi, M. Yamaguchi, J. Yokoyama, Generalized G-Inflation: Inflation with the Most General Second-Order Field Equations, Prog. Theor. Phys. 126 (2011) 511–529. doi:10.1143/PTP.126.511.

[74] M. Okounkova, Stability of Rotating Black Holes in Einstein Dilaton Gauss-Bonnet Gravity, Phys. Rev. D100 (12) (2019) 124054. doi:10.1103/PhysRevD.100.124054.

[75] C. Deffayet, O. Pujolas, I. Sawicki, A. Vikman, Imperfect Dark Energy from Kinetic Gravity Braiding, JCAP 10 (2010) 026. doi:10.1088/1475-7516/2010/10/026.

[76] T. W. Baumgarte, S. L. Shapiro, On the numerical integration of Einstein's field equations, Phys. Rev. D59 (1999) 024007. doi:10.1103/PhysRevD.59.024007.

[77] M. Shibata, T. Nakamura, Evolution of three-dimensional gravitational waves: Harmonic slicing case, Phys. Rev. D52 (1995) 5428–5444. doi:10.1103/PhysRevD.52.5428.

[78] C. Bona, J. Masso, E. Seidel, J. Stela, A New formalism for numerical relativity, Phys. Rev. Lett. 75 (1995) 600–603. doi:10.1103/PhysRevLett.75.600.

[79] S. Bernuzzi, D. Hilditch, Constraint violation in free evolution schemes: Comparing BSSNOK with a conformal decomposition of Z4, Phys. Rev. D 81 (2010) 084003. doi:10.1103/PhysRevD.81.084003.

[80] L. Andersson, V. Moncrief, Elliptic hyperbolic systems and the Einstein equations, Annales Henri Poincare 4 (2003) 1–34. doi:10.1007/s00023-003-0120-1.

[81] J. M. Martín-García, xAct: Efficient tensor computer algebra for the Wolfram Language (2002).

[82] H. R. Beyer, O. Sarbach, On the well posedness of the Baumgarte-Shapiro-Shibata-Nakamura formulation of Einstein's field equations, Phys. Rev. D 70 (2004) 104004. doi:10.1103/PhysRevD.70.104004.

[83] C. Gundlach, J. M. Martin-Garcia, Symmetric hyperbolicity and consistent boundary conditions for second order Einstein equations, Phys. Rev. D 70 (2004) 044032. doi:10.1103/PhysRevD.70.044032.

[84] E. Gourgoulhon, 3+1 Formalism in General Relativity, Vol. 846, Springer, Berlin, Heidelberg, 2012. doi:10.1007/978-3-642-24525-1.

[85] Z. Cao, D. Hilditch, Numerical stability of the Z4c formulation of general relativity, Phys. Rev. D 85 (2012) 124032. doi:10.1103/PhysRevD.85.124032.

[86] D. Hilditch, S. Bernuzzi, M. Thierfelder, Z. Cao, W. Tichy, B. Bruegmann, Compact binary evolutions with the Z4c formulation, Phys. Rev. D 88 (2013) 084057. doi:10.1103/PhysRevD.88.084057.

[87] D. Alic, C. Bona-Casas, C. Bona, L. Rezzolla, C. Palenzuela, Conformal and covariant formulation of the Z4 system with constraint-violation damping, Phys. Rev. D 85 (2012) 064040. doi:10.1103/PhysRevD.85.064040.

[88] A. Weyhausen, S. Bernuzzi, D. Hilditch, Constraint damping for the Z4c formulation of general relativity, Phys. Rev. D 85 (2012) 024038. doi:10.1103/PhysRevD.85.024038.

[89] C. Gundlach, J. M. Martin-Garcia, G. Calabrese, I. Hinder, Constraint damping in the Z4 formulation and harmonic gauge, Class. Quant. Grav. 22 (2005) 3767–3774. doi:10.1088/0264-9381/22/17/025.

[90] Y. Choquet-Bruhat, General Relativity and the Einstein Equations, Oxford Mathematical Monographs, Oxford University Press, United Kingdom, 2009.

[91] G. Nagy, O. E. Ortiz, O. A. Reula, Strongly hyperbolic second order Einstein's evolution equations, Phys. Rev. D 70 (2004) 044012. doi:10.1103/PhysRevD.70.044012.

[92] Y. Choquet-Bruhat, The Cauchy problem for stringy gravity, J. Math. Phys. 29 (1988) 1891. doi:10.1063/1.527841.

[93] C. Aragone, Stringy characteristics of effective gravity, in: SILARG 6: 6th Latin American Symposium on Relativity and Gravitation Rio de Janeiro, Brazil, July 13-18, 1987, 1987, pp. 60–69.

[94] T. Kato, Perturbation Theory for Linear Operators, Classics in Mathematics, Springer Berlin Heidelberg, Berlin, Heidelberg, 1976. doi:10.1007/978-3-642-66282-9.

[95] O. A. Reula, Strongly hyperbolic systems in general relativity, Diff. Eq. 01 (2004) 251. doi:10.1142/S0219891604000111.

[96] F. Abalos, F. Carrasco, E. Goulart, O. Reula, Nonlinear electrodynamics as a symmetric hyperbolic system, Phys. Rev. D 92 (2015) 084024. doi:10.1103/PhysRevD.92.084024.

[97] A. D. Kovacs, On the construction of asymptotically flat initial data in scalar-tensor effective field theory (3 2021). arXiv:2103.06895.

[98] G. B. Cook, Initial data for numerical relativity, Living Rev. Rel. 3 (2000) 5. doi:10.12942/lrr-2000-5.

[99] W. Tichy, The initial value problem as it relates to numerical relativity, Rept. Prog. Phys. 80 (2) (2017) 026901. doi:10.1088/1361-6633/80/2/026901.

[100] J. W. York, Jr., Conformally invariant orthogonal decomposition of symmetric tensors on Riemannian manifolds and the initial value problem of general relativity, J. Math. Phys. 14 (1973) 456–464. doi:10.1063/1.1666338.

[101] J. York, James W., Conformal 'thin sandwich' data for the initial-value problem, Phys. Rev. Lett. 82 (1999) 1350–1353. doi:10.1103/PhysRevLett.82.1350.

[102] T. W. Baumgarte, N. O. Murchadha, H. P. Pfeiffer, The Einstein constraints: Uniqueness and non-uniqueness in the conformal thin sandwich approach, Phys. Rev. D 75 (2007) 044009. doi:10.1103/PhysRevD.75.044009.

[103] J. M. Bowen, J. York, James W., Time asymmetric initial data for black holes and black hole collisions, Phys. Rev. D 21 (1980) 2047–2056. doi:10.1103/PhysRevD.21.2047.

[104] S. Brandt, B. Bruegmann, A Simple construction of initial data for multiple black holes, Phys. Rev. Lett. 78 (1997) 3606–3609. doi:10.1103/PhysRevLett.78.3606.

[105] H. P. Pfeiffer, J. York, James W., Extrinsic curvature and the Einstein constraints, Phys. Rev. D 67 (2003) 044022. doi:10.1103/PhysRevD.67.044022.

[106] M. Cantor, The existence of non-trivial asymptotically flat initial data for vacuum spacetimes, Comm. Math. Phys. 57 (1) (1977) 83–96.

[107] M. Cantor, D. Brill, The laplacian on asymptotically flat manifolds and the specification of scalar curvature, Compositio Mathematica 43 (3) (1981) 317–330.

[108] Y. Choquet-Bruhat, J. Isenberg, J. W. York, Einstein constraints on asymptotically euclidean manifolds, Phys. Rev. D 61 (2000) 084034. doi:10.1103/PhysRevD.61.084034.

[109] W. Tichy, B. Bruegmann, M. Campanelli, P. Diener, Binary black hole initial data for numerical general relativity based on post-Newtonian data, Phys. Rev. D 67 (2003) 064008. doi:10.1103/PhysRevD.67.064008.

[110] F.-L. Julié, E. Berti, $d+1$ formalism in Einstein-scalar-Gauss-Bonnet gravity, Phys. Rev. D 101 (2020) 124045. doi:10.1103/PhysRevD.101.124045.

[111] H. Witek, L. Gualtieri, P. Pani, Towards numerical relativity in scalar Gauss-Bonnet gravity: $3+1$ decomposition beyond the small-coupling limit, Phys. Rev. D 101 (12) (2020) 124055. doi:10.1103/PhysRevD.101.124055.

[112] L. Nirenberg, Topics in nonlinear functional analysis, Courant lecture notes, American Mathematical Society, Providence, RI, 2001.

[113] G. Lovelace, Reducing spurious gravitational radiation in binary-black-hole simulations by using conformally curved initial data, Classical and Quantum Gravity 26 (11) (2009) 114002. doi:10.1088/0264-9381/26/11/114002.

[114] G. B. Cook, H. P. Pfeiffer, Excision boundary conditions for black hole initial data, Phys. Rev. D 70 (2004) 104016. doi:10.1103/PhysRevD.70.104016.

[115] M. A. Scheel, H. P. Pfeiffer, L. Lindblom, L. E. Kidder, O. Rinne, S. A. Teukolsky, Solving Einstein's equations with dual coordinate frames, Phys. Rev. D 74 (2006) 104006. doi:10.1103/PhysRevD.74.104006.

[116] D. M. Walsh, Non-uniqueness in conformal formulations of the Einstein constraints, Class. Quant. Grav. 24 (2007) 1911–1926. doi:10.1088/0264-9381/24/8/002.

[117] H. P. Pfeiffer, J. W. York, Jr., Uniqueness and non-uniqueness in the Einstein constraints, Phys. Rev. Lett. 95 (2005) 091101. doi:10.1103/PhysRevLett.95.091101.

[118] M. Holst, C. Meier, Non-uniqueness of Solutions to the Conformal Formulation (10 2012).

[119] C. A. R. Herdeiro, E. Radu, H. O. Silva, T. P. Sotiriou, N. Yunes, Spin-induced scalarized black holes, Phys. Rev. Lett. 126 (1) (2021) 011103. doi:10.1103/PhysRevLett.126.011103.

[120] A. Dima, E. Barausse, N. Franchini, T. P. Sotiriou, Spin-induced black hole spontaneous scalarization, Phys. Rev. Lett. 125 (23) (2020) 231101. doi:10.1103/PhysRevLett.125.231101.

[121] E. Berti, L. G. Collodel, B. Kleihaus, J. Kunz, Spin-induced black-hole scalarization in Einstein-scalar-Gauss-Bonnet theory, Phys. Rev. Lett. 126 (1) (2021) 011104. doi:10.1103/PhysRevLett.126.011104.