Second-order perturbations of the Schwarzschild spacetime: Practical, covariant, and gauge-invariant formalisms

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High-accuracy gravitational-wave modeling demands going beyond linear, first-order perturbation theory. Particularly motivated by the need for second-order perturbative models of extreme-mass-ratio inspirals and black hole ringdowns, we present practical spherical-harmonic decompositions of the Einstein equation, Regge-Wheeler-Zerilli equations, and Teukolsky equation at second perturbative order in a Schwarzschild background. Our formulations are covariant on the t-r plane and on the two-sphere, and we express the field equations in terms of gauge-invariant metric perturbations. In a companion *Mathematica* package, PerturbationEquations, we provide these invariant formulas as well as the analogous formulas in terms of raw, gauge-dependent metric perturbations. Our decomposition of the second-order Einstein equation, when specialized to the Lorenz gauge, was a key ingredient in recent second-order self-force calculations [Phys. Rev. Lett. **124**, 021101 (2020); *ibid.* **127**, 151102 (2021); *ibid.* **130**, 241402 (2023)].

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I. INTRODUCTION

The first phase of gravitational-wave astronomy [1–3] has been a success of experimental physics, data analysis, and the theory of general relativity (GR) in its strong-field regime. It also represents a success of perturbation theory. Waveform templates commonly incorporate information from perturbative approximations, particularly from post-Newtonian theory [4], which describes the early stages of an inspiral. Many of them additionally incorporate information from black hole perturbation theory in a variety of ways. For example, effective one body models are designed to capture the point particle limit [5], in which the motion of a binary reduces to geodesic motion in a black hole spacetime; they can be informed by the associated perturbative fluxes [6–10] and by perturbative self-force corrections to black hole geodesics [11–13]; and they often use black hole perturbation theory to describe the final, ringdown phase after merger [14].

As detectors are upgraded and new detectors come online, perturbative models must be further improved. In the context of black hole perturbation theory, the overwhelming majority of calculations have been restricted to first, linear perturbative order. There are now at least two prime examples for which gravitational-wave astronomy requires going to second perturbative order, where nonlinear effects first appear. The first example is the ringdown phase of a binary [15–18]. The second is binaries with small mass ratios, such as extreme-mass-ratio inspirals (EMRIs) in which a stellar-mass compact object orbits a massive black hole [19–21].

Ringdowns have, historically, been well modeled as sums of quasinormal modes [22]. However, recent work has shown that quadratic coupling between modes can be significant and leave observable signatures in waveforms [15,16]. Any model using a perturbative treatment of ringdown will likely have to include such nonlinear effects to meet future accuracy requirements. That is especially true for models of massive black hole binaries, which will be observable (with SNRs $\sim 10^3$) by the space-based detector LISA [23].

EMRIs, which are also expected to be key sources for LISA [23], are best modeled by self-force theory, which treats the smaller object as a source of perturbations of the background spacetime of the large black hole [20,21]. It has been widely accepted for decades that accurately modeling EMRIs necessitates carrying self-force theory to second order [19,24–27]. More recently, it has been predicted that second-order self-force calculations can also provide accurate waveforms in the intermediate-mass-ratio regime and even for the mass ratios $\sim 1:10$ observable by present-day detectors [28,29]. That prediction was validated when second-order waveforms were first obtained in 2021 [30,31]. These waveforms were specialized to quasicircular, nonspinning binaries, but their high accuracy across a broad range of mass ratios (and their capacity for rapid waveform generation) provides additional motivation for extending such calculations to more generic binary configurations.

Unfortunately, although the general formulation of nonlinear perturbation theory on arbitrary backgrounds is well established [32–35], and general formulas, such as the nth-order expansion of the Einstein equation, are easily derived at any finite order [36], there has been limited development of practical, ready-at-hand tools in black hole spacetimes. Concrete calculations (e.g., [37–45]) have generally been limited to vacuum perturbations and to a small number of harmonic modes. In the simple case of a Schwarzschild background, the most thorough treatment was provided by Brizuela *et al.* [46–49], who extended the Regge-Wheeler-Zerilli (RWZ) formalism to second order. This formalism, while useful in many contexts, is limited in that it inherits the sometimes pathological behavior of the RWZ gauge [50–52] and does not provide the entire metric perturbation, missing the $\ell = 0$ and 1 modes that describe the spacetime's mass and momentum.

There is therefore call for a broader suite of tools. This is especially true for EMRIs, which bring particular complexities. In self-force calculations, the $\ell = 0$ and 1 modes of the perturbation cannot be ignored; some ingredients are only available in practical form in the Lorenz gauge [53]; and calculations often demand a large number of modes of the first-order perturbation [54] (often above $\ell = 50$).

Our goal with this paper is to provide a comprehensive, practical treatment of second-order calculations on a Schwarzschild background. Our treatment is deliberately modeled on Martel and Poisson's (hereafter MP's) now-standard summary of first-order perturbation theory in Schwarzschild [55]. Like MP, we include significant review material to make our paper a stand-alone reference. However, our treatment is more expansive than MP's, covering a wider variety of formulations to make our results useful to the broadest userbase. We also find this larger toolset provides alternative methods that are sometimes more useful than MP's at second order. In all cases, our goal is to decompose the field equations into a set of tensor or spin-weighted spherical harmonics. Our core output is a set of coupling formulas that express harmonic modes of the second-order source as sums of products of first-order field modes. We present these formulas in two forms: in terms of the gauge-dependent first- and second-order metric perturbations and in terms of gauge-invariant perturbations.

We begin in Sec. II by reviewing second-order perturbation theory in a generic vacuum background. In Secs. III and IV we specialize to a Schwarzschild background and assemble the ingredients required for the harmonic decomposition of the second-order field equations, following MP's description (with some modifications and several extensions) of the decomposition of four-dimensional covariant quantities into quantities that are separately covariant on the $t - r$ plane and on the two-sphere. Section V discusses gauge freedom at the level of harmonic modes and the construction of invariant variables. In Sec. VI, we present the decomposition of the second-order Einstein equation. Section VII then presents the decompositions of the second-order RWZ and Teukolsky equations. We conclude in Sec. VIII with a discussion of applications, specifically how our decomposition of the second-order Einstein equation underpinned the recent second-order self-force calculations in Refs. [30,56–58]. Table II and Appendix F describe how to translate our formulas into alternative choices of harmonic basis and field variables.

Alongside our paper, we provide the fully decomposed equations in a companion *Mathematica* package, PerturbationEquations, which we make available as part of the Black Hole Perturbation Toolkit [59]. The package provides utilities to work with the second-order Einstein equations, RWZ equations, and Teukolsky equations in a variety of popular harmonic bases and conventions.

II. SECOND-ORDER PERTURBATION THEORY

Before introducing any decompositions, we begin with the first- and second-order Einstein equations in their covariant, four-dimensional form on an arbitrary vacuum background spacetime, which we will specialize to Schwarzschild in later sections. We keep these formulas generic, but we write them in a form that naturally simplifies in the Lorenz gauge (the gauge used in all second-order self-force calculations to date). At the end of the section we summarize (i) the Bianchi identities that constrain the equations and (ii) the gauge freedom the equations admit.

A. Einstein equations

We write the exact spacetime metric as $\mathsf{g}_{\mu\nu} = g_{\mu\nu} + h_{\mu\nu}$, where $g_{\mu\nu}$ is the background metric and $h_{\mu\nu} \sim \epsilon \ll 1$ is a small correction, with an associated small stress-energy tensor $T_{\mu\nu} \sim \epsilon$. We will ultimately expand $h_{\mu\nu}$ and $T_{\mu\nu}$ in powers of ϵ, meaning

$$h_{\mu\nu} = \epsilon h^{(1)}_{\mu\nu} + \epsilon^2 h^{(2)}_{\mu\nu} + \mathcal{O}(\epsilon^3), \tag{1}$$

$$T_{\mu\nu} = \epsilon T^{(1)}_{\mu\nu} + \epsilon^2 T^{(2)}_{\mu\nu} + \mathcal{O}(\epsilon^3), \tag{2}$$

and write field equations for $h^{(n)}_{\mu\nu}$. But to organize those equations, we first expand curvature quantities in orders of nonlinearity in $h_{\mu\nu}$.

Explicit perturbative expressions are typically simplest when using the Einstein equation in its trace-reversed form,

$$R_{\mu\nu}[\mathsf{g}] = 8\pi \left[T_{\mu\nu} - \frac{1}{2}\mathsf{g}_{\mu\nu}(\mathsf{g}^{-1})^{\alpha\beta} T_{\alpha\beta} \right], \tag{3}$$

where $(\mathsf{g}^{-1})^{\alpha\beta}$ is the inverse of $\mathsf{g}_{\alpha\beta}$, and where we omit indices on tensorial arguments of functionals. We write the Ricci tensor's expansion in orders of nonlinearity as

$$R_{\mu\nu}[g+h]=R_{\mu\nu}[g]+\delta R_{\mu\nu}[h]+\delta^2 R_{\mu\nu}[h]+\mathcal{O}(|h_{\mu\nu}|^3), \tag{4}$$

where $\delta^n R_{\mu\nu}$ is the (normalized) nth functional derivative of $R_{\mu\nu}$, defined by

$$\delta^n R_{\mu\nu}[\varphi] \coloneqq \frac{1}{\lambda!}\frac{d^n}{d\lambda^n}R_{\mu\nu}[g+\lambda\varphi]|_{\lambda=0} \tag{5}$$

for any rank-two symmetric tensor $\varphi_{\mu\nu}$. With this definition, $\delta^n R_{\mu\nu}[h]$ is constructed from the background metric and n copies of $h_{\mu\nu}$. We use the same notation for any quantity constructed from the metric; as a trivial example, $\delta g_{\mu\nu}[h] = h_{\mu\nu}$ and $\delta^n g_{\mu\nu}[h] = 0$ for $n > 1$.

Concrete formulas for $\delta^n R_{\mu\nu}$ are found straightforwardly from the spacetime's exact Ricci tensor [60],

$$R_{\mu\nu}[g+h] = R_{\mu\nu}[g] + 2C^\rho{}_{\mu[\nu;\rho]} + 2C^\rho{}_{\sigma[\rho}C^\sigma{}_{\nu]\mu}, \tag{6}$$

where $C^\alpha{}_{\beta\gamma}$ is the exact difference between the Christoffel symbols of $\mathsf{g}_{\mu\nu}$ and $g_{\mu\nu}$. Explicitly,

$$C^\alpha{}_{\beta\gamma} = \frac{1}{2}(\mathsf{g}^{-1})^{\alpha\delta}(2h_{\delta(\beta;\gamma)} - h_{\beta\gamma;\delta}); \tag{7}$$

a semicolon and ∇ both denote the covariant derivative compatible with $g_{\alpha\beta}$. The expansion in orders of nonlinearity then immediately follows from the expansion

$$(\mathsf{g}^{-1})^{\alpha\beta} = g^{\alpha\beta} - h^{\alpha\beta} + h^\alpha{}_\gamma h^{\gamma\beta} + \mathcal{O}(|h_{\mu\nu}|^3). \tag{8}$$

Here and throughout this paper, Greek indices are lowered and raised with $g_{\mu\nu}$ and its inverse $g^{\mu\nu}$.

From Eqs. (6) and (8), and some simple manipulations (using $R_{\mu\nu}[g] = 0$), one finds

$$\delta R_{\mu\nu}[h] = -\frac{1}{2}(\mathcal{E}_{\mu\nu}[h] + \mathcal{F}_{\mu\nu}[h]), \tag{9}$$

$$\delta^2 R_{\mu\nu}[h] = \frac{1}{2}(\mathcal{A}_{\mu\nu}[h] + \mathcal{B}_{\mu\nu}[h] + \mathcal{C}_{\mu\nu}[h]), \tag{10}$$

where

$$\mathcal{E}_{\mu\nu}[h] \coloneqq \Box h_{\mu\nu} + 2R_\mu{}^\alpha{}_\nu{}^\beta h_{\alpha\beta}, \tag{11}$$

$$\mathcal{F}_{\mu\nu}[h] \coloneqq -2\bar{h}_{\alpha(\mu}{}^{;\alpha}{}_{\nu)}, \tag{12}$$

with $\Box \coloneqq g^{\mu\nu}\nabla_\mu\nabla_\nu$, and

$$\mathcal{A}_{\alpha\beta}[h] \coloneqq \frac{1}{2}h^{\mu\nu}{}_{;\alpha}h_{\mu\nu;\beta} + h^\mu{}_\beta{}^{;\nu}(h_{\mu\alpha;\nu} - h_{\nu\alpha;\mu}), \tag{13}$$

$$\mathcal{B}_{\alpha\beta}[h] \coloneqq -h^{\mu\nu}(2h_{\mu(\alpha;\beta)\nu} - h_{\alpha\beta;\mu\nu} - h_{\mu\nu;\alpha\beta}), \tag{14}$$

$$\mathcal{C}_{\alpha\beta}[h] \coloneqq -\bar{h}^{\mu\nu}{}_{;\nu}(2h_{\mu(\alpha;\beta)} - h_{\alpha\beta;\mu}). \tag{15}$$

We use an overbar to denote trace reversal with the background metric, as in $\bar{h}_{\mu\nu} \coloneqq h_{\mu\nu} - \frac{1}{2}g_{\mu\nu}g^{\alpha\beta}h_{\alpha\beta}$.

If we now substitute Eqs. (4) and (8) into the exact Einstein equation (3), along with the series expansions (1) and (2), then we can equate coefficients of powers of ϵ. The result is the sequence of linear equations

$$\delta R_{\mu\nu}[h^{(1)}] = 8\pi\mathcal{T}^{(1)}_{\mu\nu}, \tag{16}$$

$$\delta R_{\mu\nu}[h^{(2)}] = 8\pi\mathcal{T}^{(2)}_{\mu\nu} - \delta^2 R_{\mu\nu}[h^{(1)}], \tag{17}$$

with matter source terms

$$\mathcal{T}^{(1)}_{\mu\nu} = \bar{T}^{(1)}_{\mu\nu}, \tag{18}$$

$$\mathcal{T}^{(2)}_{\mu\nu} = \bar{T}^{(2)}_{\mu\nu} - \frac{1}{2}\left(h^{(1)}_{\mu\nu}g^{\alpha\beta} - g_{\mu\nu}h^{(1)\alpha\beta}\right)T^{(1)}_{\alpha\beta}. \tag{19}$$

In the Lorenz gauge, where $\bar{h}^{\mu\nu}{}_{;\nu} = 0$, the quantities $\mathcal{C}_{\mu\nu}$ and $\mathcal{F}_{\mu\nu}$ both vanish, simplifying the field equations to

$$\mathcal{E}_{\mu\nu}[h^{(1)}] = -16\pi\mathcal{T}^{(1)}_{\mu\nu}, \tag{20}$$

$$\mathcal{E}_{\mu\nu}[h^{(2)}] = -16\pi\mathcal{T}^{(2)}_{\mu\nu} + \mathcal{A}_{\mu\nu}[h^{(1)}] + \mathcal{B}_{\mu\nu}[h^{(1)}]. \tag{21}$$

Alternatively, we can write the field equations in terms of the perturbed Einstein tensor. The analogs of Eqs. (16) and (17) are

$$\delta G_{\mu\nu}[h^{(1)}] = 8\pi T^{(1)}_{\mu\nu}, \tag{22}$$

$$\delta G_{\mu\nu}[h^{(2)}] = 8\pi T^{(2)}_{\mu\nu} - \delta^2 G_{\mu\nu}[h^{(1)}]. \tag{23}$$

The perturbations of $G_{\mu\nu}$ are immediately obtained from those of $R_{\mu\nu}$ using $\delta^n G_{\mu\nu} = \delta^n(R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}g^{\alpha\beta}R_{\alpha\beta})$. In a Ricci-flat background, this simplifies to

$$\delta G_{\mu\nu} = \overline{\delta R}_{\mu\nu}, \tag{24}$$

$$\delta^2 G_{\mu\nu} = \overline{\delta^2 R}_{\mu\nu} - \frac{1}{2}(h_{\mu\nu}g^{\alpha\beta} - g_{\mu\nu}h^{\alpha\beta})\delta R_{\alpha\beta}. \tag{25}$$

In vacuum regions, where $\delta R_{\mu\nu}[h^{(1)}] = 0 = T^{(1)}_{\mu\nu}$, $\mathcal{T}^{(2)}_{\mu\nu}$ reduces to $\bar{T}^{(2)}_{\mu\nu}$ and $\delta^2 G_{\mu\nu}[h^{(1)}]$ reduces to $\overline{\delta^2 R}_{\mu\nu}[h^{(1)}]$.

We write the field equations (16) and (17) in generic form as

$$\delta R_{\mu\nu}[h^{(n)}] = \bar{S}^{(n)}_{\mu\nu}. \tag{26}$$

The relations (24) and (25) ensure that field equations in the form (16) and (17) can be written in terms of a trace reversal with respect to the background metric,

$$\delta G_{\mu\nu}[h^{(n)}] = S^{(n)}_{\mu\nu}, \tag{27}$$

where $S^{(n)}_{\mu\nu} := \bar{S}^{(n)}_{\mu\nu} - \frac{1}{2} g_{\mu\nu} g^{\alpha\beta} \bar{S}^{(n)}_{\alpha\beta}$. In the Lorenz gauge,

$$\mathcal{E}_{\mu\nu}[h^{(n)}] = -2\bar{S}^{(n)}_{\mu\nu} \tag{28}$$

and

$$\mathcal{E}_{\mu\nu}[\bar{h}^{(n)}] = -2S^{(n)}_{\mu\nu}, \tag{29}$$

where we have used the fact that $\bar{\mathcal{E}}_{\mu\nu}[h] = \mathcal{E}_{\mu\nu}[\bar{h}]$.

For simplicity, in the paper we only provide the harmonic decompositions of quantities appearing in Eq. (26) [and therefore also Eq. (28)]. The companion package PerturbationEquations additionally includes the decompositions of $\delta G_{\mu\nu}$ and $\delta^2 G_{\mu\nu}$.

B. Bianchi identities and conservation equations

The components of the perturbative Einstein equations are not all independent. They are related by the contracted Bianchi identity $(\mathsf{g}^{-1})^{\beta\gamma}\,{}^{\mathsf{g}}\nabla_\gamma G_{\alpha\beta}[\mathsf{g}] = 0$, where ${}^{\mathsf{g}}\nabla_\alpha$ is the covariant derivative compatible with $\mathsf{g}_{\alpha\beta}$. Expanding that identity in orders of nonlinearity, we obtain the identities

$$g^{\beta\gamma}\nabla_\gamma \delta G_{\alpha\beta} = 0, \tag{30}$$

$$g^{\beta\gamma}\nabla_\gamma \delta^2 G_{\alpha\beta} = h^{\beta\gamma}\nabla_\gamma \delta G_{\alpha\beta} + 2\delta C^{\gamma\beta}{}_{(\alpha}\delta G_{\beta)\gamma}. \tag{31}$$

Here $\delta C^{\alpha}{}_{\beta\gamma}[h] := \frac{1}{2} g^{\alpha\delta}(2\nabla_{(\beta}h_{\gamma)\delta} - \nabla_\delta h_{\beta\gamma})$ is the linear perturbation of the Christoffel symbol. These identities hold for any symmetric rank-two tensor $h_{\alpha\beta}$.

By virtue of the field equations, these identities are equivalent to stress-energy conservation $(\mathsf{g}^{-1})^{\beta\gamma}\,{}^{\mathsf{g}}\nabla_\gamma T_{\alpha\beta} = 0$, or

$$\nabla^\beta T^{(1)}_{\alpha\beta} = 0, \tag{32}$$

$$\nabla^\beta T^{(2)}_{\alpha\beta} = h^{(1)\beta\gamma}\nabla_\gamma T^{(1)}_{\alpha\beta} + 2\delta C^{\gamma\beta}{}_{(\alpha}T^{(1)}_{\beta)\gamma}. \tag{33}$$

Since Eq. (30) holds for any $h_{\alpha\beta}$, it immediately implies that the sources $S^{(n)}_{\alpha\beta}$ appearing in the field equations (27) must all be conserved with respect to the background divergence,

$$\nabla^\beta S^{(n)}_{\alpha\beta} = 0. \tag{34}$$

C. Gauge freedom

Perturbation theory in GR comes with well-known gauge freedom corresponding to the choice of how to identify points on the exact spacetime with points in the background spacetime [34,61,62]; see Sec. IVA of Ref. [63] or Appendix A of this paper for a concise summary. To understand the practical consequence of this, let $A = A^{(0)} + \epsilon A^{(1)} + \epsilon^2 A^{(2)} + \mathcal{O}(\epsilon^3)$ be the expansion of a generic tensor of arbitrary rank (in index-free notation). Under a gauge transformation, the terms in this expansion transform as $A^{(n)} \to A^{(n)} + \Delta A^{(n)}$, where

$$\Delta A^{(1)} = \mathcal{L}_{\xi_{(1)}} A^{(0)}, \tag{35a}$$

$$\Delta A^{(2)} = \mathcal{L}_{\xi_{(2)}} A^{(0)} + \frac{1}{2}\mathcal{L}^2_{\xi_{(1)}} A^{(0)} + \mathcal{L}_{\xi_{(1)}} A^{(1)}. \tag{35b}$$

Here $\mathcal{L}$ denotes a Lie derivative, and the gauge generators $\xi^\mu_{(n)}$ correspond to the small coordinate transformation

$$x'^\mu = x^\mu - \epsilon\xi^\mu_{(1)}(x) - \epsilon^2\left[\xi^\mu_{(2)}(x) - \frac{1}{2}\xi^\nu_{(1)}(x)\partial_\nu \xi^\mu_{(1)}(x)\right] + \mathcal{O}(\epsilon^3). \tag{36}$$

Applying Eq. (35) to the metric perturbations $h^{(n)}_{\mu\nu}$ yields

$$\Delta h^{(1)}_{\mu\nu} = \mathcal{L}_{\xi_{(1)}} g_{\mu\nu}, \tag{37a}$$

$$\Delta h^{(2)}_{\mu\nu} = \mathcal{L}_{\xi_{(2)}} g_{\mu\nu} + \frac{1}{2}\mathcal{L}^2_{\xi_{(1)}} g_{\mu\nu} + \mathcal{L}_{\xi_{(1)}} h^{(1)}_{\mu\nu}. \tag{37b}$$

Applying it to the stress-energy tensor in a vacuum background yields

$$\Delta T^{(1)}_{\mu\nu} = 0, \tag{38a}$$

$$\Delta T^{(2)}_{\mu\nu} = \mathcal{L}_{\xi_{(1)}} T^{(1)}_{\mu\nu}. \tag{38b}$$

The field equations (16) and (17) are invariant under a generic gauge transformation, as can be established from the above transformation laws and the identities [63]

$$\Delta\delta R_{\mu\nu}[h^{(1)}] = 0, \tag{39}$$

$$\Delta\delta R_{\mu\nu}[h^{(2)}] = \delta R_{\mu\nu}[\Delta h^{(2)}], \tag{40}$$

$$\Delta\delta^2 R_{\mu\nu}[h^{(1)}] = \mathcal{L}_{\xi_{(1)}}\delta R_{\mu\nu}[h^{(1)}] - \delta R_{\mu\nu}\left[\frac{1}{2}\mathcal{L}^2_{\xi_{(1)}} g\right] - \delta R_{\mu\nu}[\mathcal{L}_{\xi_{(1)}} h^{(1)}]. \tag{41}$$

Analogous equations apply for the transformation of $\delta^n G_{\mu\nu}$.

We stress that, while the second-order field equation (17) is invariant, the individual terms in it are not. In particular, the left-hand side of (17) has the nontrivial transformation (40), while the sources on the right-hand side have the nontrivial transformations (38b) and (41). This differs from the situation at first order, where (in a vacuum background) Eqs. (38a) and (39) ensure that each side of the field equation is separately invariant.

III. TENSORS AND BASES ON $\mathcal{M}^2 \times S^2$

When specialized to a Schwarzschild background, the perturbative Einstein equations are fully separable by virtue of the background's stationarity and spherical symmetry. The spherical symmetry allows us to naturally decompose 4D tensorial quantities into $2+2$D quantities. Specifically, we follow MP in writing the spacetime manifold $\mathcal{M}$ as the Cartesian product $\mathcal{M} = \mathcal{M}^2 \times S^2$, where $\mathcal{M}^2$ is the "t-r plane" and S^2 is the two-sphere. This method, which is generally attributed to Gerlach and Sengupta [64], enables us to work with quantities that are separately covariant on $\mathcal{M}^2$ and S^2. Tensors on S^2 are then naturally decomposed into harmonics.

Although we mostly follow MP, we do adopt slightly different notation. Table I provides the conversion between the two.

A. Covariant decompositions

We let x^a be coordinates on $\mathcal{M}^2$ and give tensors on $\mathcal{M}^2$ lowercase Latin indices $a, b, c, \ldots$; analogously, we let θ^A be coordinates on S^2 and give tensors on S^2 uppercase Latin indices $A, B, C, \ldots$. The background line element can then be written as

$$ds^2 = g_{ab}dx^a dx^b + r^2\Omega_{AB}d\theta^A d\theta^B, \tag{42}$$

where r is the areal radius of a sphere of fixed x^a, g_{ab} is the restriction of $g_{\mu\nu}$ to $\mathcal{M}^2$, and Ω_{AB} is the metric of the unit sphere. We use g_{ab} and its inverse g^{ab} to lower and raise indices of tensors on $\mathcal{M}^2$, and Ω_{AB} and its inverse Ω^{AB} to lower and raise indices of tensors on S^2. We also require the Levi-Civita tensors ϵ_{ab} and ϵ_{AB}. In standard polar coordinates $\theta^A = (\theta, \phi)$, the tensors on S^2 are given by

$$\Omega_{AB} = \mathrm{diag}(1, \sin^2\theta) \quad \text{and} \quad \epsilon_{\theta\phi} = \sin\theta = -\epsilon_{\phi\theta}. \tag{43}$$

Decomposing the field equations (16) and (17) into tensors on $\mathcal{M}^2$ and S^2 requires doing likewise for covariant derivatives. We define δ_a and D_A to be the derivatives compatible with g_{ab} and Ω_{AB}, respectively, with corresponding Christoffel symbols $\Gamma[\delta]^a_{bc}$ and $\Gamma[D]^A_{BC}$. The nonvanishing Christoffel symbols $\Gamma^\mu_{\nu\rho}$ associated with ∇_α are related to these according to $\Gamma^a_{bc} = \Gamma[\delta]^a_{bc}$, $\Gamma^A_{BC} = \Gamma[D]^A_{BC}$, and

$$\Gamma^a_{AB} = -rr^a\Omega_{AB}, \qquad \Gamma^A_{Bc} = \frac{\delta^A_B r_c}{r}, \tag{44}$$

where

$$r_a \coloneqq \partial_a r. \tag{45}$$

This allows us to decompose the components of a derivative $\nabla_\alpha v^\beta$ into covariant quantities on $\mathcal{M}^2$ and S^2:

$$\nabla_a v^b = \delta_a v^b, \tag{46a}$$

$$\nabla_a v^B = \delta_a v^B + r^{-1}r_a v^B, \tag{46b}$$

$$\nabla_A v^b = D_A v^b - rr^b\Omega_{AB}v^B, \tag{46c}$$

$$\nabla_A v^B = D_A v^B + r^{-1}\delta^B_A r_c v^c, \tag{46d}$$

where D_A acts on v^b as it would on a scalar, and δ_a acts on v^B as it would on a scalar. Similarly, the components of $\nabla_\alpha\omega_\beta$ are written as

$$\nabla_a\omega_b = \delta_a\omega_b, \tag{47a}$$

$$\nabla_a\omega_B = \delta_a\omega_B - r^{-1}r_a\omega_B, \tag{47b}$$

$$\nabla_A\omega_b = D_A\omega_b - r^{-1}\omega_A r_b, \tag{47c}$$

$$\nabla_A\omega_B = D_A\omega_B + r\Omega_{AB}r^c\omega_c. \tag{47d}$$

Higher derivatives are expressed in the same manner.

We will also require the Riemann tensors associated with the derivatives δ_a and D_A, $R[\delta]_{abcd}$ and $R[D]_{ABCD}$. They are given by

$$R[\delta]_{abcd} = \frac{2M}{r^3}(g_{ac}g_{bd} - g_{ad}g_{bc}), \tag{48}$$

$$R[D]_{ABCD} = \Omega_{AC}\Omega_{BD} - \Omega_{AD}\Omega_{BC}. \tag{49}$$

In concrete calculations, our first step is always to expand contractions into $2+2$D form and then project any free indices onto either $\mathcal{M}^2$ or $\mathcal{S}^2$. For example,

$$g^{\alpha\beta}\nabla_\alpha h_{\beta\gamma} = g^{ab}\nabla_a h_{b\gamma} + r^{-2}\Omega^{AB}\nabla_A h_{B\gamma}. \tag{50}$$

Choosing $\gamma = c$ (i.e., projecting onto $\mathcal{M}^2$) and then using Eq. (47), one obtains a fully decomposed expression:

$$g^{\alpha\beta}\nabla_\alpha h_{\beta c} = g^{ab}\delta_a h_{bc} + r^{-2}\Omega^{AB}D_A h_{Bc} + 2r^{-1}r^a h_{ac} - r^{-3}h^A{}_A r_c, \tag{51}$$

where $h^A{}_A = \Omega^{AB}h_{AB}$.

TABLE I. Relationship between our bases and derivatives and those of Martel and Poisson (MP) [55].

This paper	MP
t_a	$-f^{-1}t^{MP}_a$
r_a	r_a
δ_a	∇_a
D_A	D_A

B. Bases on $\mathcal{M}^2$ and S^2

Most of our results will be fully covariant, without any choice of basis on $\mathcal{M}^2$ or S^2. However, we will on occasion adopt specific bases.

1. Bases on $\mathcal{M}^2$

As a coordinate basis for tensors on $\mathcal{M}^2$, we use (t_a, r_a), where r_a is defined in Eq. (45) and

$$t_a := \partial_a t. \tag{52}$$

Here t is the usual Schwarzschild time, and we note that MP use the same notation to instead denote the timelike Killing vector; the two are related by $t^a = -f^{-1} t^a_{MP}$, with

$$f = (-t^a t_a)^{-1} = r^a r_a = 1 - \frac{2M}{r}. \tag{53}$$

In terms of these quantities, we have

$$g_{ab} = -f t_a t_b + f^{-1} r_a r_b, \tag{54}$$

$$\epsilon_{ab} = t_a r_b - r_a t_b. \tag{55}$$

We will also make use of a Newman-Penrose null basis

$$l^a = \frac{\gamma}{\sqrt{2f}}(1, f), \tag{56}$$

$$n^a = \frac{1}{\sqrt{2f}\gamma}(1, -f), \tag{57}$$

where the components are given in (t, r) coordinates and $\gamma = \gamma(r) > 0$ is an arbitrary boost factor. This basis satisfies $l^a n_a = -1$ and $l^a l_a = 0 = n^a n_a$, which imply

$$g_{ab} = -l_a n_b - n_a l_b, \tag{58}$$

$$\epsilon_{ab} = l_a n_b - n_a l_b, \tag{59}$$

and

$$l^b \delta_b l^a = l^a \delta_b l^b, \qquad n^b \delta_b n^a = n^a \delta_b n^b,$$
$$l^b \delta_b n^a = -n^a \delta_b l^b, \qquad n^b \delta_b l^a = -l^a \delta_b n^b. \tag{60}$$

The divergences that appear in (60) are given by

$$\delta_a l^a = \frac{r^2 f \partial_r \gamma + M\gamma}{r^2 \sqrt{2f}} \quad \text{and} \quad \delta_a n^a = \frac{r^2 f \partial_r \gamma - M\gamma}{r^2 \sqrt{2f}\gamma^2}. \tag{61}$$

In the definition of the null basis vectors, the boost factor γ is commonly chosen to be one of the following [21,65–67]:

$$\text{Carter}: \gamma = 1, \tag{62a}$$

$$\text{Kinnersley}: \gamma = \sqrt{2/f}, \tag{62b}$$

$$\text{Hartle-Hawking}: \gamma = \sqrt{f/2}. \tag{62c}$$

In the Kinnersley basis, $\delta_a l^a = 0$; in the Hartle-Hawking basis, $\delta_a n^a = 0$; in the Carter basis, $\delta_a l^a = -\delta_a n^a \neq 0$. In the Kinnersley basis, l^a is tangent to affinely parametrized outgoing null rays, where r is the affine parameter. This makes the Kinnersley basis singular at the future horizon but particularly useful for studying outgoing radiation: in retarded Eddington-Finkelstein coordinates (u, r),

$$l^a_{\rm K}\partial_a = \partial_r \quad \text{and} \quad n^a_{\rm K}\partial_a = \partial_u - (f/2)\partial_r. \tag{63}$$

In the Hartle-Hawking basis, n^a is tangent to affinely parametrized ingoing null rays, where r is again the affine parameter. This makes the Hartle-Hawking basis singular at the past horizon but particularly useful for studying ingoing radiation: in advanced Eddington-Finkelstein coordinates (v, r),

$$l^a_{\rm HH}\partial_a = \partial_v + (f/2)\partial_r \quad \text{and} \quad n^a_{\rm HH}\partial_a = -\partial_r. \tag{64}$$

The Carter basis is singular at both the past and future horizon, but it has the advantage of maintaining a symmetry between ingoing and outgoing null directions: in double null coordinates (u, v),

$$l^a_{\rm C}\partial_a = \sqrt{\frac{2}{f}}\partial_v \quad \text{and} \quad n^a_{\rm C}\partial_a = \sqrt{\frac{2}{f}}\partial_u. \tag{65}$$

2. Bases on S^2

As a basis on S^2, we define a complex null vector

$$\tilde{m}^A = \left(1, \frac{i}{\sin\theta}\right) \tag{66}$$

and its complex conjugate, $\tilde{m}^{A*}$, where the components are given in (θ, ϕ) coordinates. Our definition of $\tilde{m}^A$ differs by a factor of $\sqrt{2}r$ relative to the traditional Newman-Penrose basis [68]. With our choice of normalization, the basis vectors satisfy

$$\tilde{m}^A \tilde{m}_A = 0, \qquad \tilde{m}^B D_B \tilde{m}^A = \tilde{m}^A D_B \tilde{m}^B,$$
$$\tilde{m}^A \tilde{m}^*_A = 2, \qquad \tilde{m}^{B*} D_B \tilde{m}^A = -\tilde{m}^A D_B \tilde{m}^{B*}, \tag{67}$$

and

$$\Omega_{AB} = \frac{1}{2}(\tilde{m}_A \tilde{m}^*_B + \tilde{m}^*_A \tilde{m}_B), \tag{68}$$

$$\epsilon_{AB} = \frac{i}{2}(\tilde{m}_A \tilde{m}^*_B - \tilde{m}^*_A \tilde{m}_B). \tag{69}$$

In (θ, ϕ) coordinates,

$$D_B \tilde{m}^B = D_B \tilde{m}^{B*} = \cot\theta. \tag{70}$$

Equation (69) also provides the useful identity

$$\epsilon^A_B \tilde{m}^B = i\tilde{m}^A. \tag{71}$$

It will be useful to also define the Newman-Penrose basis,

$$m^A = \frac{1}{\sqrt{2}r}\tilde{m}^A, \tag{72}$$

which satisfies $g_{AB}m^A m^{B*} = 1$, and in terms of which

$$g_{AB} = r^4(m_A m_B^* + m_A^* m_B). \tag{73}$$

The factor of r^4 arises from the fact that indices are lowered with Ω_{AB}.

The set of vectors $\{l^\alpha, n^\alpha, m^\alpha, m^{\alpha*}\}$ forms a null tetrad on $\mathcal{M}$, with the natural definitions $l^A = n^A = m^a = 0$. A generic symmetric tensor $h_{\alpha\beta}$ can be decomposed into this basis according to

$$h_{ab} = h_{ll}n_a n_b + h_{ln}(n_a l_b + l_a n_b) + h_{nn}l_a l_b, \tag{74a}$$

$$h_{aA} = -r^2 h_{lm} n_a m_A^* - r^2 h_{nm} l_a m_A^* + \text{c.c.}, \tag{74b}$$

$$h_{AB} = r^4 h_{mm} m_A^* m_B^* + r^4 h_{mm^*} m_A^* m_B + \text{c.c.} \tag{74c}$$

Alternatively, we can decompose it in a mixed basis $\{t_a, r_a, \tilde{m}_A, \tilde{m}_A^*\}$, according to

$$h_{ab} = h_{tt}t_a t_b + h_{tr}(t_a r_b + r_a t_b) + h_{rr}r_a r_b, \tag{75a}$$

$$h_{aA} = \frac{1}{2}(h_{t\tilde{m}}t_a\tilde{m}_A^* + h_{r\tilde{m}}r_a\tilde{m}_A^* + \text{c.c.}), \tag{75b}$$

$$h_{AB} = \frac{1}{4}(h_{\tilde{m}\tilde{m}}\tilde{m}_A^*\tilde{m}_B^* + h_{\tilde{m}\tilde{m}^*}\tilde{m}_A^*\tilde{m}_B + \text{c.c.}), \tag{75c}$$

or only partially decompose it, according to

$$h_{ab} = h_{tt}t_a t_b + h_{tr}(t_a r_b + r_a t_b) + h_{rr}r_a r_b, \tag{76a}$$

$$h_{aB} = h_{tB}t_a + h_{rB}r_a, \tag{76b}$$

$$h_{AB} = h_{AB}. \tag{76c}$$

As a final comment, we observe the main practical advantage of working with the quantities $\{g_{ab}, \delta_a, \Omega_{AB}, D_A\}$. Besides allowing tensor-harmonic decompositions while preserving invariance, these choices enforce that the background quantities on $\mathcal{M}^2$ commute with those on S^2:

$$D_A g_{ab} = \delta_a \Omega_{AB} = [D_A, \delta_a] = 0. \tag{77}$$

This is not the case if working with g_{AB} and ∇_A. Likewise, $\tilde{m}^A$ often provides a more convenient basis than m^A because

$$\delta_a \tilde{m}^A = [l, \tilde{m}] = [n, \tilde{m}] = 0. \tag{78}$$

In this last equation, $[\cdot,\cdot]$ denotes the vector commutator, $[u,v]^\alpha \coloneqq u^\beta\partial_\beta v^\alpha - v^\beta\partial_\beta u^\alpha = u^\beta\nabla_\beta v^\alpha - v^\beta\nabla_\beta u^\alpha = \mathcal{L}_u v^\alpha$.

By working with trivially commuting quantities, our choices (like MP's) take maximal advantage of Schwarzschild's spherical symmetry.

IV. DECOMPOSITIONS INTO SPIN-WEIGHTED AND TENSOR SPHERICAL HARMONICS

The literature contains numerous bases of spherical harmonics that can be used to decompose the field equations. With the exception of the Teukolsky formalism, calculations in Schwarzschild spacetime typically use tensor harmonic bases. For that reason, we will decompose the metric perturbation and Einstein equations into tensor harmonics, specifically adopting MP's choice of harmonics. However, for reasons explained below, instead of tensor harmonics we take spin-weighted spherical harmonics ${}_sY_{lm}$ to be the "base" harmonics. Our expansions in tensor harmonics will utilize spin-weighted harmonics as an intermediary. This will also allow us to easily connect to the Teukolsky formalism in Sec. VII B. We refer to Brizuela *et al.* for a treatment that consistently uses tensor harmonics rather than spin-weighted ones [46–48].

Given the large number of common conventions for harmonic expansions, in Table II we provide translations between conventions.

A. Spin-weighted harmonics

A spin-weighted tensor v on S^2 is said to have spin weight s if it transforms as $v \to e^{is\varphi}v$ under the complex phase rotation $\tilde{m}^A \to e^{i\varphi}\tilde{m}^A$ [68]. In practice, this means v's spin weight is the number of factors of $\tilde{m}^A$ appearing in it minus the number of factors of $\tilde{m}^{A*}$ appearing in it.

We define derivative operators

$$ð = \tilde{m}^A D_A - s(D_A\tilde{m}^A), \tag{79a}$$

$$ð' = \tilde{m}^{A*} D_A + s(D_A\tilde{m}^{A*}), \tag{79b}$$

which act on tensors of spin-weight s. Our definitions and notation here differ slightly from common conventions in the literature, as summarized in Table III. The derivative ð raises the spin weight by 1, while ð′ lowers it by 1. They satisfy the Leibniz rule [e.g., $ð(uv) = (ðu)v + uðv$, where u and v can have differing spin weights], and the identities (67) ensure they annihilate $\tilde{m}^A$ and $\tilde{m}^{A*}$:

$$ð\tilde{m}^A = ð'\tilde{m}^A = ð\tilde{m}^{A*} = ð'\tilde{m}^{A*} = 0. \tag{80}$$

They satisfy the commutation and anticommutation relations

$$\frac{1}{2}(ð'ð - ðð') = i\epsilon^{AB}D_A D_B + s, \tag{81a}$$

$$\frac{1}{2}(ð'ð + ðð') = D_A D^A + s[(D_B m^{B*})m^A D_A - \text{c.c.}] - s^2|D_A\tilde{m}^A|^2. \tag{81b}$$

When acting on a spin-weighted scalar (such as a component h_{am}), they satisfy $ð^i ð'^j = ð'^j ð^i$ if $j = i + 2s$.

TABLE II. Relationship between harmonic coefficients in various conventions. The relationship between the tensorial and tetrad decompositions is the same for sources (bottom half of table) as for metric perturbations (top half of table). Additional relations can be found in Eq. (112) and Appendix F of this paper and Table I of Ref. [21].

This paper (tensorial)	Martel and Poisson [55]	This paper (tetrad)	Barack-Lousto-Sago [69,70]
$h^{\ell m}_{ab}$	$h^{\ell m}_{ab}$	$l_a l_b h^{\ell m}_{nn} + 2l_{(a}n_{b)}h^{\ell m}_{ln} + n_a n_b h^{\ell m}_{ll}$	$\frac{1}{2r}[(\bar{h}_{1\ell m} + f\bar{h}_{6\ell m})t_a t_b + f^{-1}\bar{h}_{2\ell m}(t_a r_b + r_a t_b) + f^{-2}(\bar{h}_{1\ell m} - f\bar{h}_{6\ell m})r_a r_b]$
$h^{\ell m}_{a+}$	$j^{\ell m}_a$	$\frac{r}{\sqrt{2}\lambda_{\ell,1}}[l_a(h^{\ell m}_{nm} - h^{\ell m}_{nm^*}) + n_a(h^{\ell m}_{lm} - h^{\ell m}_{lm^*})]$	$\frac{1}{2\lambda^2_{\ell,1}}(\bar{h}_{4\ell m}t_a + f^{-1}\bar{h}_{5\ell m}r_a)$
$h^{\ell m}_{+}$	$r^2 G^{\ell m}$	$\frac{r^2}{\lambda_{\ell,2}}(h^{\ell m}_{mm} + h^{\ell m}_{m^*m^*})$	$\frac{r}{\lambda^2_{\ell,2}}\bar{h}_{7\ell m}$
$h^{\ell m}_{\circ}$	$r^2 K^{\ell m}$	$r^2 h^{\ell m}_{mm^*}$	$\frac{r}{2}\bar{h}_{3\ell m}$
$h^{\ell m}_{a-}$	$h^{\ell m}_a$	$-\frac{ir}{\sqrt{2}\lambda_{\ell,1}}[l_a(h^{\ell m}_{nm} + h^{\ell m}_{nm^*}) + n_a(h^{\ell m}_{lm} + h^{\ell m}_{lm^*})]$	$-\frac{1}{2\lambda^2_{\ell,1}}(\bar{h}_{8\ell m}t_a + f^{-1}\bar{h}_{9\ell m}r_a)$
$h^{\ell m}_{-}$	$h^{\ell m}_2$	$-\frac{ir^2}{\lambda_{\ell,2}}(h^{\ell m}_{mm} - h^{\ell m}_{m^*m^*})$	$-\frac{r}{\lambda^2_{\ell,2}}\bar{h}_{10\ell m}$
$S^{\ell m}_{ab}$	$Q^{\ell m}_{ab}$	$\vdots$	$\frac{1}{\sqrt{2}}[(S_{1\ell m} + fS_{3\ell m})t_a t_b + f^{-1}S_{2\ell m}(t_a r_b + r_a t_b) + f^{-2}(S_{1\ell m} - fS_{3\ell m})r_a r_b]$
$S^{\ell m}_{a+}$	$\frac{1}{2}Q^{\ell m}_a$	$\vdots$	$\frac{r}{\sqrt{2}\lambda_{\ell,1}}(S_{4\ell m}t_a + f^{-1}S_{5\ell m}r_a)$
$S^{\ell m}_{+}$	$\frac{1}{2}Q^{\sharp}_{\ell m}$	$\vdots$	$\frac{\sqrt{2}r^2}{\lambda_{\ell,2}}S_{7\ell m}$
$S^{\ell m}_{\circ}$	$\frac{r^2}{2}Q^{\flat}_{\ell m}$	$\vdots$	$\frac{r^2}{\sqrt{2}}S_{6\ell m}$
$S^{\ell m}_{a-}$	$\frac{1}{2}P^{\ell m}_a$	$\vdots$	$-\frac{r}{\sqrt{2}\lambda_{\ell,1}}(S_{8\ell m}t_a + f^{-1}S_{9\ell m}r_a)$
$S^{\ell m}_{-}$	$P^{\ell m}$	$\vdots$	$-\frac{\sqrt{2}r^2}{\lambda_{\ell,2}}S_{10\ell m}$

Like D_A, they commute with background quantities on $\mathcal{M}^2$:

$$\eth g_{ab} = \eth' g_{ab} = [\delta_a, \eth] = [\delta_a, \eth'] = 0. \tag{82}$$

A spin-weighted scalar of spin-weight s is conveniently expanded as a sum of spin-weighted spherical harmonics of the same spin weight, defined for $\ell \geq |s|$ as

$${}_sY_{\ell m} \coloneqq \frac{1}{\lambda_{\ell,s}}\begin{cases} (-1)^s \eth^s Y_{\ell m}, & 0 \leq s \leq \ell, \\ \eth'^{|s|} Y_{\ell m}, & -\ell \leq s \leq 0, \end{cases} \tag{83}$$

where

$$\lambda_{\ell,s} \coloneqq \sqrt{\frac{(\ell + |s|)!}{(\ell - |s|)!}} = \sqrt{(l - |s| + 1)_{2|s|}}. \tag{84}$$

We also define for later use the related quantity μ_ℓ by

$$\mu^2_\ell \coloneqq (\ell + 2)(\ell - 1) = (\lambda_{\ell,2}/\lambda_{\ell,1})^2 = \lambda^2_{\ell,1} - 2. \tag{85}$$

Here we adopt standard definitions; these are precisely the spin-weighted harmonics defined by Newman and Penrose [68], simply reexpressed in terms of our convention for the operators $\eth$ and $\eth'$. These definitions are also consistent with, for example, *Mathematica*'s `SphericalHarmonicY` function and with the `SpinWeightedSphericalHarmonicY` function in the Black Hole Perturbation toolkit's `SpinWeightedSphericalHarmonicY` package [59,73]. Note that although Goldberg *et al.* [74] is also a standard reference for the spin-weighted spherical

TABLE III. Relationship between our derivatives and those of Newman and Penrose (NP) [68,71] and Geroch-Held-Penrose (GHP) [72]. We note that Ref. [21] adopts GHP conventions. The quantities β, ρ, ϵ, and $\gamma_{\rm NP}$ appearing in the relations are Newman-Penrose spin coefficients, which in our context reduce to $\beta = \frac{1}{2}D_A m^A$; $\rho = -l^a r_a F r$; $\epsilon = \frac{1}{2}\delta_a l^a = \frac{1}{2}\partial_r l^r$; and $\gamma_{\rm NP} = -\frac{1}{2}\delta_a n^a = -\frac{1}{2}\partial_r n^r$, or $\gamma_{\rm NP} = -\epsilon'$ in GHP notation. The quantity b is boost weight, defined above Eq. (196a).

This paper	NP [71]	NP [68]	GHP
$\eth$	$\sqrt{2}r(\boldsymbol{\delta} - 2s\beta)$	$-\eth_{\rm NP}$	$\sqrt{2}r\eth_{\rm GHP}$
$\eth'$	$\sqrt{2}r(\bar{\boldsymbol{\delta}} + 2s\beta)$	$-\bar{\eth}_{\rm NP}$	$\sqrt{2}r\eth'_{\rm GHP}$
Þ	$\boldsymbol{D} - 2b\epsilon$	$\vdots$	Þ
Þ′	$\boldsymbol{\Delta} - 2b\gamma_{\rm NP}$	$\vdots$	Þ′

harmonics, their definition includes a nonstandard overall factor of $(-1)^m$.

The spin-weighted harmonics are related to Wigner D matrices (again, following conventions consistent with *Mathematica*'s `WignerD` function) according to

$$ {}_sY_{\ell m}(\theta,\phi) = (-1)^s\sqrt{\frac{2\ell+1}{4\pi}}D^{\ell}_{-sm}(0,\theta,\phi). \tag{86}$$

They satisfy the orthonormality conditions

$$\oint {}_sY^*_{\ell m}\,{}_sY_{\ell' m'}d\Omega = \delta_{\ell\ell'}\delta_{mm'}, \tag{87}$$

where $d\Omega = \sin\theta d\theta d\phi$, and they have the properties [74]

$$ {}_sY^*_{\ell m} = (-1)^{m+s}\,{}_{-s}Y_{\ell,-m}, \tag{88a}$$

$$ \eth\,{}_sY_{\ell m} = -\sqrt{(\ell-s)(\ell+s+1)}\,{}_{s+1}Y_{\ell m}, \tag{88b}$$

$$ \eth'\,{}_sY_{\ell m} = \sqrt{(\ell+s)(\ell-s+1)}\,{}_{s-1}Y_{\ell m}, \tag{88c}$$

$$ \eth'\eth\,{}_sY_{\ell m} = -(\ell-s)(\ell+s+1)\,{}_sY_{\ell m}. \tag{88d}$$

Because of our sign convention for ð, Eqs. (88b) and (88c) differ by an overall sign relative to the analogous formulas in Ref. [74]. The identity (88d) is an eigenvalue equation that can equivalently be written as

$$\frac{1}{2}(\eth\eth' + \eth'\eth)\,{}_sY_{\ell m} = -[\ell(\ell+1)-s^2]\,{}_sY_{\ell m}. \tag{89}$$

Spin-weighted harmonics are convenient for two key reasons. First, Eq. (17) involves many derivatives, and any number of covariant derivatives of $Y_{\ell m}$ can be easily written in terms of ${}_sY_{\ell m}$. For example, using $D_AY_{\ell m} = \frac{1}{2}(\tilde m_A\tilde m^{B*} + \tilde m^*_A\tilde m^B)D_BY_{\ell m}$ together with Eqs. (79) and (88), one finds

$$D_AY_{\ell m} = \frac{\lambda_{\ell,1}}{2}({}_{-1}Y_{\ell m}\tilde m_A - {}_1Y_{\ell m}\tilde m^*_A). \tag{90}$$

Doing the same for $D_AD_BY_{\ell m}$ and making use of Eqs. (67), (79), and (88), one finds

$$\begin{aligned} D_AD_BY_{\ell m} = {}& \frac{\lambda_{\ell,2}}{4}({}_{-2}Y_{\ell m}\tilde m_A\tilde m_B + {}_2Y_{\ell m}\tilde m^*_A\tilde m^*_B) \\ & - \frac{\lambda^2_{\ell,1}}{2}Y_{\ell m}\Omega_{AB}. \end{aligned} \tag{91}$$

Higher derivatives are given in Eqs. (C2) and (C3).

The second reason spin-weighted harmonics are useful is that, when one expands the first-order field in a basis of harmonics, the sources in Eq. (17) involve products of those harmonics, and decomposing that product into a sum of single harmonics requires the integral of three harmonics. With spin-weighted harmonics, that integral is easily found. We define the desired integral as

$$C^{\ell ms}_{\ell' m' s'\ell'' m'' s''} := \oint {}_sY^*_{\ell m s'}Y_{\ell' m' s''}Y_{\ell'' m''}d\Omega. \tag{92}$$

For $s = s' + s''$, one can explicitly evaluate the integral using Eq. (86) and then following Sec. 30B of Ref. [75] to derive the integral of three Wigner D matrices. The result is [76]

$$\begin{aligned} C^{\ell ms}_{\ell' m' s'\ell'' m'' s''} = {}& (-1)^{m+s}\sqrt{\frac{(2\ell+1)(2\ell'+1)(2\ell''+1)}{4\pi}} \\ & \times\begin{pmatrix}\ell & \ell' & \ell'' \\ s & -s' & -s''\end{pmatrix}\begin{pmatrix}\ell & \ell' & \ell'' \\ -m & m' & m''\end{pmatrix}, \end{aligned} \tag{93}$$

where the arrays are $3j$ symbols. It follows from the symmetries of the $3j$ symbol that

$$C^{\ell ms}_{\ell' m' s'\ell'' m'' s''} = (-1)^{\ell+\ell'+\ell''}C^{\ell m-s}_{\ell' m'-s'\ell'' m''-s''}, \tag{94a}$$

$$C^{\ell ms}_{\ell' m' s'\ell'' m'' s''} = (-1)^{\ell+\ell'+\ell''}C^{\ell -ms}_{\ell' -m' s'\ell'' -m'' s''}, \tag{94b}$$

$$C^{\ell ms}_{\ell' m' s'\ell'' m'' s''} = C^{\ell ms}_{\ell'' m'' s''\ell' m' s'}. \tag{94c}$$

It also follows that the usual rules associated with coupling of angular momenta are enforced, since the $C^{\ell ms}_{\ell' m' s'\ell'' m'' s''}$ are zero unless

$$m = m' + m'', \tag{95a}$$

$$|\ell' - \ell''| \le \ell \le \ell' + \ell''. \tag{95b}$$

Finally, we note that for $\ell = m = s = 0$ and $s'' = -s'$, the result collapses to

$$C^{000}_{\ell' m' s'\ell'' m'' s''} = \frac{(-1)^{m'+s'}}{\sqrt{4\pi}}\delta_{\ell'\ell''}\delta_{m',-m''}. \tag{96}$$

To decompose Eq. (17) in tensor harmonics, we will express all quantities in terms of spin-weighted harmonics. Equation (93) then becomes the essential tool in the decomposition. To the best of our knowledge, this strategy has not appeared in prior literature.

B. Tensor harmonics

Tensor harmonics of rank s are constructed from symmetric and trace-free combinations of covariant derivatives of ordinary scalar harmonics $Y_{\ell m}$ [46][1]:

$$Y^{\ell m}_{A_1\cdots A_s} := D_{\langle A_1}\cdots D_{A_s\rangle}Y_{\ell m}, \tag{97a}$$

$$X^{\ell m}_{A_1\cdots A_s} := -\epsilon_{\langle A_1}{}^{C}D_{A_2}\cdots D_{A_s\rangle}D_CY_{\ell m}, \tag{97b}$$

[1]To maintain compatibility with MP, we have introduced a minus sign into Ref. [46]'s definition of $X^{\ell m}_{A_1\cdots A_s}$.

where angular brackets denote the symmetric-trace-free part of a tensor, with traces defined using Ω^{AB}. These harmonics are defined only for $\ell \geq s$, as they identically vanish for $0 \leq \ell < s$. They are related to spin-weighted harmonics by the simple formulas

$$Y^{\ell m}_{A_1\cdots A_s} = \frac{\lambda_{\ell,s}}{2^s}[{}_{-s}Y_{\ell m}\tilde{m}_{A_1}\cdots\tilde{m}_{A_s} + (-1)^s{}_sY_{\ell m}\tilde{m}^*_{A_1}\cdots\tilde{m}^*_{A_s}], \tag{98a}$$

$$X^{\ell m}_{A_1\cdots A_s} = -\frac{i\lambda_{\ell,s}}{2^s}[{}_{-s}Y_{\ell m}\tilde{m}_{A_1}\cdots\tilde{m}_{A_s} - (-1)^s{}_sY_{\ell m}\tilde{m}^*_{A_1}\cdots\tilde{m}^*_{A_s}]; \tag{98b}$$

see Appendix C. The harmonics $Y_{\ell m}$ and $Y^{\ell m}_{A_1\cdots A_s}$ are said to have even parity, transforming as $Y^{\ell m}_{A_1\cdots A_s} \to (-1)^\ell Y^{\ell m}_{A_1\cdots A_s}$ under the parity inversion $(\theta,\phi)\to(\pi-\theta,\phi+\pi)$, while $X^{\ell m}_{A_1\cdots A_s}$ are said to have odd parity, transforming as $X^{\ell m}_{A_1\cdots A_s} \to (-1)^{\ell+1}X^{\ell m}_{A_1\cdots A_s}$. In the linearized field equations, the even- and odd-parity sectors decouple. However, at second order they couple through the source terms in the field equation (17).

Brizuela *et al.* [46–48] worked consistently with tensor harmonics rather than spin-weighted ones, motivating their use of rank-$s > 2$ harmonics. However, in our case we will only require rank-one (vector) and rank-two tensor harmonics. Specializing Eq. (97) to these cases, we see that the vector harmonics, defined for $\ell \geq 1$, are given by

$$Y^{\ell m}_A \coloneqq D_A Y_{\ell m}, \tag{99a}$$

$$X^{\ell m}_A \coloneqq -\epsilon_A{}^C D_C Y_{\ell m}, \tag{99b}$$

and the tensor harmonics, defined for $\ell \geq 2$, are given by

$$Y^{\ell m}_{AB} \coloneqq \left[D_A D_B + \frac{1}{2}\ell(\ell+1)\Omega_{AB}\right]Y_{\ell m}, \tag{100a}$$

$$X^{\ell m}_{AB} \coloneqq -\epsilon_{(A}{}^C D_{B)} D_C Y_{\ell m}. \tag{100b}$$

In the formula for $Y^{\ell m}_{AB}$, we have used the eigenvalue equation

$$D_A D^A Y_{\ell m} = -\ell(\ell+1)Y_{\ell m}. \tag{101}$$

By construction, the tensor harmonics are trace free:

$$\Omega^{AB}Y^{\ell m}_{AB} = 0 = \Omega^{AB}X^{\ell m}_{AB}. \tag{102}$$

From Eq. (98), they are related to spin-weighted harmonics as

$$Y^{\ell m}_A = \frac{\lambda_{\ell,1}}{2}({}_{-1}Y_{\ell m}\tilde{m}_A - {}_1Y_{\ell m}\tilde{m}^*_A), \tag{103a}$$

$$X^{\ell m}_A = -\frac{\lambda_{\ell,1}}{2}i({}_{-1}Y_{\ell m}\tilde{m}_A + {}_1Y_{\ell m}\tilde{m}^*_A), \tag{103b}$$

$$Y^{\ell m}_{AB} = \frac{\lambda_{\ell,2}}{4}({}_{-2}Y_{\ell m}\tilde{m}_A\tilde{m}_B + {}_2Y_{\ell m}\tilde{m}^*_A\tilde{m}^*_B), \tag{103c}$$

$$X^{\ell m}_{AB} = -\frac{\lambda_{\ell,2}}{4}i({}_{-2}Y_{\ell m}\tilde{m}_A\tilde{m}_B - {}_2Y_{\ell m}\tilde{m}^*_A\tilde{m}^*_B). \tag{103d}$$

They are orthogonal with respect to the natural inner product on S^2, but they are not orthonormal:

$$\oint Y^{A*}_{\ell m}Y^{\ell' m'}_A d\Omega = \lambda^2_{\ell,1}\delta_{\ell\ell'}\delta_{mm'}, \tag{104a}$$

$$\oint X^{A*}_{\ell m}X^{\ell' m'}_A d\Omega = \lambda^2_{\ell,1}\delta_{\ell\ell'}\delta_{mm'}, \tag{104b}$$

$$\oint Y^{AB*}_{\ell m}Y^{\ell' m'}_{AB} d\Omega = \frac{\lambda^2_{\ell,2}}{2}\delta_{\ell\ell'}\delta_{mm'}, \tag{104c}$$

$$\oint X^{AB*}_{\ell m}X^{\ell' m'}_{AB} d\Omega = \frac{\lambda^2_{\ell,2}}{2}\delta_{\ell\ell'}\delta_{mm'}, \tag{104d}$$

and

$$\oint X^{A*}_{\ell m}Y^{\ell' m'}_A d\Omega = 0 = \oint X^{AB*}_{\ell m}Y^{\ell' m'}_{AB} d\Omega. \tag{105}$$

C. Harmonic expansions

In terms of the MP harmonics, any symmetric tensor $v_{\mu\nu}$ can be expanded as

$$v_{ab} = \sum_{\ell m} v^{\ell m}_{ab}Y_{\ell m}, \tag{106a}$$

$$v_{aA} = \sum_{\ell m}(v^{\ell m}_{a+}Y^{\ell m}_A + v^{\ell m}_{a-}X^{\ell m}_A), \tag{106b}$$

$$v_{AB} = \sum_{\ell m}(v^{\ell m}_{\circ}\Omega_{AB}Y^{\ell m} + v^{\ell m}_{+}Y^{\ell m}_{AB} + v^{\ell m}_{-}X^{\ell m}_{AB}), \tag{106c}$$

where the coefficients are functions of x^a. Here and throughout this paper, sums range over all allowed values of ℓ and m. If $v_{\mu\nu}$ is real valued, then all of its harmonic coefficients satisfy

$$v^{\ell,-m}_{\cdot} = (-1)^m v^{\ell m*}_{\cdot}. \tag{107}$$

Here and below we use the following shorthand.

Definition. A dot, as in $v^{\ell m}_{\cdot}$, is used to denote a generic tensor-harmonic coefficient, in this case any of $v^{\ell m}_{ab}$, $v^{\ell m}_{a\pm}$, $v^{\ell m}_{\pm}$, or $v^{\ell m}_{\circ}$.

Our convention in Eq. (106) differs slightly from that of MP, who followed tradition [77] by introducing a factor of r^2 in front of $v^{\ell m}_{\circ}$ and $v^{\ell m}_{+}$. Our notation also differs from tradition in that we uniformly use a "+" sign to denote the coefficient of an even-parity vector or tensor harmonic, a

"−" sign to denote the coefficient of an odd-parity vector or tensor harmonic, and a "∘" to denote one-half the angular trace of a tensor.

Using the orthogonality of the harmonics, each of the coefficients in Eq. (106) can be written as an integral against the appropriate harmonic:

$$v^{lm}_{ab} = \oint v_{ab} Y^*_{lm} d\Omega, \tag{108a}$$

$$v^{lm}_{a+} = \frac{1}{\lambda^2_{\ell,1}} \oint v_{aA} Y^{A*}_{lm} d\Omega, \tag{108b}$$

$$v^{lm}_{a-} = \frac{1}{\lambda^2_{\ell,1}} \oint v_{aA} X^{A*}_{lm} d\Omega, \tag{108c}$$

$$v^{lm}_{\circ} = \frac{1}{2} \oint v_{AB} \Omega^{AB} Y^*_{lm} d\Omega, \tag{108d}$$

$$v^{lm}_{+} = \frac{2}{\lambda^2_{\ell,2}} \oint v_{AB} Y^{AB*}_{lm} d\Omega, \tag{108e}$$

$$v^{lm}_{-} = \frac{2}{\lambda^2_{\ell,2}} \oint v_{AB} X^{AB*}_{lm} d\Omega. \tag{108f}$$

To facilitate use of Eq. (93), in practice we express these as integrals against spin-weighted harmonics using the relations (103).

These expansions in tensor harmonics are covariant; they do not depend on any choice of basis vectors on S^2. If we adopt the null basis $\{m^A, m^{A*}\}$ on S^2, then components of a symmetric tensor $v_{\mu\nu}$ can instead be expanded in spin-weighted harmonics according to

$$v_{ab} = \sum_{\ell m} v^{\ell m}_{ab} Y_{\ell m}, \tag{109a}$$

$$v_{am} = \sum_{\ell m} v^{\ell m}_{am\,1} Y_{\ell m}, \tag{109b}$$

$$v_{am^*} = \sum_{\ell m} v^{\ell m}_{am^*\,-1} Y_{\ell m}, \tag{109c}$$

$$v_{mm} = \sum_{\ell m} v^{\ell m}_{mm\,2} Y_{\ell m}, \tag{109d}$$

$$v_{m^*m^*} = \sum_{\ell m} v^{\ell m}_{m^*m^*\,-2} Y_{\ell m}, \tag{109e}$$

$$v_{mm^*} = \sum_{\ell m} v^{\ell m}_{mm^*} Y_{\ell m}. \tag{109f}$$

In these expansions, the spin weights are carried by the harmonics; the coefficients have spin weight 0.

If $v_{\mu\nu}$ is real, then $v_{am^*} = (v_{am})^*$ and $v_{m^*m^*} = (v_{mm})^*$. Together with Eq. (88a), this implies

$$v^{\ell,-m}_{am} = -(-1)^m (v^{\ell m}_{am^*})^*, \tag{110a}$$

$$v^{\ell,-m}_{mm} = (-1)^m (v^{\ell m}_{m^*m^*})^*. \tag{110b}$$

More generally, the modes of a spin-weight s scalar, $v = \sum_{\ell m} v_{\ell m s} Y_{\ell m}$, are related to the modes of its complex conjugate, $v^* = \sum_{\ell m} v^*_{\ell m -s} Y_{\ell m}$, by

$$v^*_{\ell m} = (-1)^{m+s} (v^{\ell,-m})^*. \tag{111}$$

The coefficients in the spin-weighted harmonic decomposition are easily related to those in Eq. (106):

$$v^{\ell m}_{am} = -\frac{\lambda_{\ell,1}}{\sqrt{2}r}(v^{\ell m}_{a+} + i v^{\ell m}_{a-}), \tag{112a}$$

$$v^{\ell m}_{am^*} = \frac{\lambda_{\ell,1}}{\sqrt{2}r}(v^{\ell m}_{a+} - i v^{\ell m}_{a-}), \tag{112b}$$

$$v^{\ell m}_{mm} = \frac{\lambda_{\ell,2}}{2r^2}(v^{\ell m}_{+} + i v^{\ell m}_{-}), \tag{112c}$$

$$v^{\ell m}_{m^*m^*} = \frac{\lambda_{\ell,2}}{2r^2}(v^{\ell m}_{+} - i v^{\ell m}_{-}), \tag{112d}$$

$$v^{\ell m}_{mm^*} = \frac{1}{r^2} v^{\ell m}_{\circ}. \tag{112e}$$

We conclude with the explicit expansion of our main quantity of interest: the metric perturbation. Its expansion reads

$$h_{ab} = \sum_{\ell m} h^{\ell m}_{ab} Y^{\ell m}, \tag{113a}$$

$$h_{aA} = \sum_{\ell m} (h^{\ell m}_{a+} Y^{\ell m}_A + h^{\ell m}_{a-} X^{\ell m}_A), \tag{113b}$$

$$h_{AB} = \sum_{\ell m} (h^{\ell m}_{\circ} \Omega_{AB} Y^{\ell m} + h^{\ell m}_{+} Y^{\ell m}_{AB} + h^{\ell m}_{-} X^{\ell m}_{AB}). \tag{113c}$$

We will likewise write the decomposition of a generic source term in the Einstein equations (27) as

$$S_{ab} = \sum_{\ell m} S^{\ell m}_{ab} Y^{\ell m}, \tag{114a}$$

$$S_{aA} = \sum_{\ell m} (S^{\ell m}_{a+} Y^{\ell m}_A + S^{\ell m}_{a-} X^{\ell m}_A), \tag{114b}$$

$$S_{AB} = \sum_{\ell m} (S^{\ell m}_{\circ} \Omega_{AB} Y^{\ell m} + S^{\ell m}_{+} Y^{\ell m}_{AB} + S^{\ell m}_{-} X^{\ell m}_{AB}). \tag{114c}$$

The field equations also often involve the trace reversal of these fields, $\bar{h}_{\mu\nu}$ and $\bar{S}_{\mu\nu}$. To facilitate trace reversals at the level of harmonic coefficients, for a generic field $v_{\mu\nu}$ we introduce

$$v_{\bullet}^{\ell m} \coloneqq \frac{1}{2} g^{ab} v_{ab}^{\ell m} \tag{115}$$

in analogy with $v_{\circ}^{\ell m}$. The coefficients in the tensor-harmonic expansion of $\bar{v}_{\mu\nu} \coloneqq v_{\mu\nu} - \frac{1}{2} g_{\mu\nu} g^{\alpha\beta} v_{\alpha\beta}$ are then related to those in the expansion of $v_{\mu\nu}$ by

$$\bar{v}_{ab}^{\ell m} = v_{ab}^{\ell m} - g_{ab}(v_{\bullet}^{\ell m} + r^{-2} v_{\circ}^{\ell m}), \tag{116a}$$

$$\bar{v}_{\circ}^{\ell m} = -r^2 v_{\bullet}^{\ell m}, \tag{116b}$$

$$\bar{v}_{a\pm}^{\ell m} = v_{a\pm}^{\ell m} \quad \text{and} \quad \bar{v}_{\pm}^{\ell m} = v_{\pm}^{\ell m}. \tag{116c}$$

If instead we expand $v_{\mu\nu}$ and $\bar{v}_{\mu\nu}$ in spin-weighted harmonics, then

$$\bar{v}_{ln}^{\ell m} = v_{mm^*}^{\ell m} \quad \text{and} \quad \bar{v}_{mm^*}^{\ell m} = v_{ln}^{\ell m}, \tag{117}$$

and all other coefficients satisfy $\bar{v}_{\cdot}^{\ell m} = v_{\cdot}^{\ell m}$.

V. GAUGE TRANSFORMATIONS AND INVARIANT PERTURBATIONS

In Ref. [55], MP wrote the first-order Einstein equation in terms of a set of gauge-invariant metric perturbations. Here we extend that approach to second order. In the accompanying PerturbationEquations package, we also provide the second-order field equations in terms of the original, gauge-dependent perturbations. We discuss the relative merits of each approach at the end of the section.

A. Gauge transformations of harmonic coefficients

We first examine how tensor-harmonic coefficients transform under a change of gauge. That requires decomposing Eq. (37), which in turn requires the decompositions of Lie derivatives. Consider the Lie derivative $\mathcal{L}_\xi v_{\mu\nu}$ of a symmetric tensor $v_{\mu\nu}$ along a vector $\xi^\mu = (\zeta^a, Z^A)$. It has components

$$(\mathcal{L}_\xi v)_{ab} = l_\zeta v_{ab} + \pounds_Z v_{ab} + 2 v_{C(a} \delta_{b)} Z^C, \tag{118a}$$

$$(\mathcal{L}_\xi v)_{aB} = l_\zeta v_{aB} + \pounds_Z v_{aB} + v_{BC} \delta_a Z^C + v_{ac} D_B \zeta^c, \tag{118b}$$

$$(\mathcal{L}_\xi v)_{AB} = l_\zeta v_{AB} + \pounds_Z v_{AB} + 2 v_{c(A} D_{B)} \zeta^c, \tag{118c}$$

where l_ζ is a Lie derivative on $\mathcal{M}^2$, and $\pounds_Z$ is a Lie derivative on S^2. We can use the decomposition (118) to calculate the components of $\Delta h_{\mu\nu}^{(1)}$ straightforwardly from Eq. (37a). Given that result, we may then use the decomposition (118) a second time to calculate the components of $\Delta h_{\mu\nu}^{(2)}$, after rewriting Eq. (37b) as

$$\Delta h_{\mu\nu}^{(2)} = \mathcal{L}_{\xi_{(2)}} g_{\mu\nu} + H_{\mu\nu} \tag{119}$$

with

$$H_{\mu\nu} \coloneqq \mathcal{L}_{\xi_{(1)}} \left(h_{\mu\nu}^{(1)} + \frac{1}{2} \Delta h_{\mu\nu}^{(1)} \right). \tag{120}$$

To obtain the harmonic expansion of the result, we expand $\xi_{(n)}^\mu$ in vector harmonics as

$$\zeta_{(n)}^a = \sum_{\ell m} \zeta_{(n)\ell m}^a Y_{\ell m}, \tag{121a}$$

$$Z_{(n)}^A = \sum_{\ell m} (Z_{(n)\ell m}^+ Y_{\ell m}^A + Z_{(n)\ell m}^- X_{\ell m}^A), \tag{121b}$$

where, recall, $Y_{\ell m}^A \coloneqq \Omega^{AB} Y_B^{\ell m}$ and $X_{\ell m}^A \coloneqq \Omega^{AB} X_B^{\ell m}$.

For the first-order transformation $\Delta h_{\mu\nu}^{(1)} = \mathcal{L}_{\xi_{(1)}} g_{\mu\nu}$, Eq. (118) reduces to

$$\Delta h_{ab}^{(1)} = 2\delta_{(a} \zeta_{b)}^{(1)}, \tag{122a}$$

$$\Delta h_{aB}^{(1)} = r^2 \delta_a Z_B^{(1)} + D_B \zeta_a^{(1)}, \tag{122b}$$

$$\Delta h_{AB}^{(1)} = 2 r r_c \zeta_{(1)}^c \Omega_{AB} + 2 r^2 D_{(A} Z_{B)}^{(1)}. \tag{122c}$$

Substituting the harmonic expansion (121) into Eq. (122), one finds

$$\Delta h_{ab}^{(1)\ell m} = 2\delta_{(a} \zeta_{b)}^{(1)\ell m}, \tag{123a}$$

$$\Delta h_{a+}^{(1)\ell m} = r^2 \delta_a Z_+^{(1)\ell m} + \zeta_a^{(1)\ell m}, \tag{123b}$$

$$\Delta h_{a-}^{(1)\ell m} = r^2 \delta_a Z_-^{(1)\ell m}, \tag{123c}$$

$$\Delta h_{\circ}^{(1)\ell m} = 2 r r_c \zeta_{(1)\ell m}^c - \ell(\ell+1) r^2 Z_+^{(1)\ell m}, \tag{123d}$$

$$\Delta h_{\pm}^{(1)\ell m} = 2 r^2 Z_{\pm}^{(1)\ell m}. \tag{123e}$$

In the same way, the harmonic decomposition of Eq. (119) reads

$$\Delta h_{ab}^{(2)\ell m} = 2\delta_{(a} \zeta_{b)}^{(2)\ell m} + H_{ab}^{\ell m}, \tag{124a}$$

$$\Delta h_{a+}^{(2)lm} = r^2 \delta_a Z_+^{(2)\ell m} + \zeta_a^{(2)\ell m} + H_{a+}^{\ell m}, \tag{124b}$$

$$\Delta h_{a-}^{(2)lm} = r^2 \delta_a Z_-^{(2)\ell m} + H_{a-}^{\ell m}, \tag{124c}$$

$$\Delta h_{\circ}^{(2)lm} = 2 r r_c \zeta_{(2)\ell m}^c - \ell(\ell+1) r^2 Z_+^{(2)\ell m} + H_{\circ}^{\ell m}, \tag{124d}$$

$$\Delta h_{\pm}^{(2)lm} = 2 r^2 Z_{\pm}^{(2)\ell m} + H_{\pm}^{\ell m}. \tag{124e}$$

The mode decompositions of the quadratic quantity $H_{\alpha\beta}$ are obtained through the following steps:

(1) Write Eq. (120) in $2+2$D form using Eq. (118).
(2) Substitute the harmonic expansions of $h^{(1)}_{\alpha\beta}$ and $\xi^\alpha_{(1)}$.
(3) Use Eqs. (90), (91), (99), (100), (C2), and (C3) to express tensor harmonics and their covariant derivatives as sums of spin-weighted harmonics.
(4) Use Eq. (108) to pick out the tensor-harmonic coefficients of the result.
(5) Use Eq. (92) to express the result in terms of the constants $C^{\ell m s}_{\ell' m' s' \ell'' m'' s''}$.
(6) Use the symmetries (94) and relabel summation indices to minimize the number of constants $C^{\ell m s}_{\ell' m' s' \ell'' m'' s''}$.

This gives us the final expressions:

$$H^{\ell m}_{ab} = \sum_{\substack{\ell' m' \ell'' m'' \\ s'=0,1}} \lambda_{\ell',s'}\lambda_{\ell'',s'} C^{\ell m 0}_{\ell' m' s' \ell'' m'' -s'} H^{\ell' m' s' \ell'' m'' -s'}_{ab}, \tag{125a}$$

$$H^{\ell m}_{a\pm} = \sum_{\substack{\ell' m' \ell'' m'' \\ s'=1,2}} \frac{\lambda_{\ell',s'}\lambda_{\ell'',1-s'}}{\lambda_{\ell,1}} C^{\ell m 1}_{\ell' m' s' \ell'' m'',1-s'} H^{\ell' m' s' \ell'' m'',1-s'}_{a\pm}, \tag{125b}$$

$$H^{\ell m}_{\circ} = \sum_{\substack{\ell' m' \ell'' m'' \\ s'=0,1,2}} \lambda_{\ell',s'}\lambda_{\ell'',s'} C^{\ell m 0}_{\ell' m' s' \ell'' m'' -s'} H^{\ell' m' s' \ell'' m'' -s'}_{\circ}, \tag{125c}$$

$$H^{\ell m}_{\pm} = \sum_{\substack{\ell' m' \ell'' m'' \\ s'=1,2,3}} \frac{\lambda_{\ell',s'}\lambda_{\ell'',2-s'}}{\lambda_{\ell,2}} C^{\ell m 2}_{\ell' m' s' \ell'' m'',2-s'} H^{\ell' m' s' \ell'' m'',2-s'}_{\pm}, \tag{125d}$$

where the quantities $H^{\ell' m' s' \ell'' m'' s''}_{\cdot}$ are made up of quadratic products of first-order mode coefficients $h^{(1)\ell' m'}_{\cdot}$, $h^{(1)\ell'' m''}_{\cdot}$, $\zeta^a_{(1)\ell' m'}$, $\zeta^a_{(1)\ell'' m''}$, $Z^\pm_{(1)\ell' m'}$, and $Z^\pm_{(1)\ell'' m''}$. We give those products, which we refer to as coupling functions, explicitly in Eq. (D2).

Equation (125) has the appearance of a quintuple sum

$$\sum_{\ell'=0}^{\infty}\sum_{\ell''=0}^{\infty}\sum_{m'=-\ell'}^{+\ell'}\sum_{m''=-\ell''}^{+\ell''}\sum_{s'=0}^{s'_{\max}}. \tag{126}$$

However, these summation ranges are restricted by the factors $C^{\ell m s}_{\ell' m' s' \ell'' m'' s''}$, which enforce the conditions in Eq. (95). The definitions of tensor harmonics also automatically enforce $\ell' \geq s'$ and we additionally require $s = s' + s''$. Together these restrictions reduce the sums to

$$\sum_{s'=0}^{s'_{\max}}\sum_{\ell'=s'}^{\infty}\sum_{\ell''=\max(|s-s'|,\,|\ell-\ell'|)}^{\ell+\ell'}\sum_{m'=-\ell'}^{+\ell'} \delta_{m'',m-m'}. \tag{127}$$

B. Common gauge choices

There are several common gauge conditions in Schwarzschild spacetime. These include the RWZ gauge [77,78], the ingoing and outgoing radiation gauges (IRG and ORG), and the Lorenz gauge:

$$\text{RWZ:}\ h_{mm} = 0 = (h_{am} - h_{am^*}). \tag{128a}$$

$$\text{IRG:}\ h_{\alpha\beta}l^\beta = 0 = g^{\alpha\beta}h_{\alpha\beta}. \tag{128b}$$

$$\text{ORG:}\ h_{\alpha\beta}n^\beta = 0 = g^{\alpha\beta}h_{\alpha\beta}. \tag{128c}$$

$$\text{Lorenz:}\ \nabla^\beta \bar{h}_{\alpha\beta} = 0. \tag{128d}$$

Here and below, we do not distinguish between $h^{(1)}_{\alpha\beta}$ and $h^{(2)}_{\alpha\beta}$. The gauge conditions can be applied to either or both of them, and one can "mix and match" by adopting a different condition for $h^{(2)}_{\alpha\beta}$ than for $h^{(1)}_{\alpha\beta}$.

The RWZ gauge is the most common because it greatly simplifies the field equations. Following MP, we will make extensive use of it in the sections below.

The radiation gauges, which reduce to so-called light-cone gauges [37,79] for specific choices of null basis, are particularly useful for studying ingoing or outgoing radiation. If the Kinnersley tetrad is used, then the IRG condition ensures that radially outgoing null cones have the same coordinate description in the perturbed spacetime as in the background spacetime: surfaces of constant retarded time u are null cones, and r is an affine parameter along the generators of the cones. If the Hartle-Hawking tetrad is used, then the ORG condition ensures that the analogous statements apply to ingoing null cones.[2] The radiation gauges also ensure that r remains an areal radius in the perturbed spacetime. This follows from the fact that if $h_{\alpha\beta}l^\beta = 0$ or $h_{\alpha\beta}n^\beta = 0$, then the traceless condition $g^{\alpha\beta}h_{\alpha\beta} = 0$ is equivalent to $\Omega^{AB}h_{AB} = 0$; since $\Omega^{AB}h_{AB}$ is proportional to the perturbation of the area element on the sphere of constant r, the surface area of the sphere remains $4\pi r^2$.

Finally, the Lorenz gauge condition is useful for putting the perturbative field equations in the symmetric hyperbolic form [(20) and (21)].

[2]The traditional names and geometrical features of the radiation gauge conditions may appear antithetical: the *outgoing* radiation gauge preserves *ingoing* null cones, which should make it ideal for studying ingoing waves, while the *ingoing* radiation gauge preserves *outgoing* null cones, which should make it ideal for studying outgoing waves. This clash stems from the particular metric reconstruction method traditionally used to obtain the metric perturbation in these gauges, reviewed in Sec. VII B below. Despite the geometrical features of the gauge conditions, the reconstruction method yields metric perturbations that match the gauges' names: outgoing (ingoing) radiation is asymptotically regular in the ORG (IRG), while ingoing (outgoing) radiation is asymptotically irregular in the ORG (IRG) [80].

In mode-decomposed form, the gauge conditions become

$$\text{RWZ:}\ h^{\ell m}_{\pm} = h^{\ell m}_{a+} = 0. \tag{129a}$$

$$\text{IRG:}\ \begin{cases} h^{\ell m}_{la} = h^{\ell m}_{l\pm} = 0, \\ h^{\ell m}_{\circ} = 0. \end{cases} \tag{129b}$$

$$\text{ORG:}\ \begin{cases} h^{\ell m}_{na} = h^{\ell m}_{n\pm} = 0, \\ h^{\ell m}_{\circ} = 0. \end{cases} \tag{129c}$$

$$\text{Lorenz:}\ \begin{cases} \delta^b \bar{h}^{\ell m}_{ab} = \frac{1}{r^3}(\lambda^2_{\ell,1} r \bar{h}^{\ell m}_{a+} + 2r_a \bar{h}^{\ell m}_{\circ} - 2r^2 r^b \bar{h}^{\ell m}_{ab}), \\ \delta^b \bar{h}^{\ell m}_{b+} = \frac{1}{2r^2}(\mu^2_\ell \bar{h}^{\ell m}_{+} - 4rr^b \bar{h}^{\ell m}_{b+} - 2\bar{h}^{\ell m}_{\circ}), \\ \delta^b \bar{h}^{\ell m}_{b-} = \frac{1}{2r^2}(\mu^2_\ell \bar{h}^{\ell m}_{-} - 4rr^b \bar{h}^{\ell m}_{b-}), \end{cases} \tag{129d}$$

where μ_ℓ is defined in Eq. (85). Note that MP denote this same quantity as μ, meaning $\mu_{\rm MP} = \mu^2_\ell$.

All four conditions leave residual gauge freedom, meaning in each case one can find gauge perturbations $\nabla_{(\alpha}\xi_{\beta)}$ that satisfy the relevant gauge conditions. Specifically, the RWZ gauge condition does not constrain $\ell = 0$ modes or the $\ell = 1$ mode h^{1m}_{a-}; the radiation gauges can be altered by a gauge vector satisfying $l^\beta \nabla_{(\alpha}\xi_{\beta)} = 0$ (IRG) or $n^\beta \nabla_{(\alpha}\xi_{\beta)} = 0$ (ORG) and $\nabla_\alpha \xi^\alpha = 0$; and the Lorenz gauge can be altered by a gauge vector satisfying $\nabla^\beta \overline{\nabla_{(\alpha}\xi_{\beta)}} = 0$ (which is equivalent to $\Box \xi^\alpha = 0$). In the next sections, we will specifically analyze (and remove) the gauge freedom in the $\ell = 0$, 1 modes.

C. Gauge-fixing procedure and residual gauge freedom

It is common in perturbation theory to construct gauge-invariant metric perturbations using a gauge-fixing procedure; see, for example, Refs. [47,48,55,81–85] and Nakamura's recent series of papers exploring this method in Schwarzschild spacetime [86–90]. The idea is to identify gauge conditions that completely fix the gauge, leaving no residual gauge freedom. The gauge vectors, call them $\tilde{\xi}^\mu_{(n)}$, that transform from a generic gauge to the fixed gauge are then determined by the perturbations in the generic gauge, call them $h^{(n)}_{\mu\nu}$. Referring to the transformation rule (37), we can then construct gauge-invariant perturbations $\tilde{h}^{(n)}_{\mu\nu}$ that are simply the metric perturbations in the fixed gauge expressed in terms of the perturbations $h^{(n)}_{\mu\nu}$ in the generic gauge:

$$\tilde{h}^{(1)}_{\mu\nu} = h^{(1)}_{\mu\nu} + \mathcal{L}_{\tilde{\xi}_{(1)}} g_{\mu\nu}, \tag{130a}$$

$$\tilde{h}^{(2)}_{\mu\nu} = h^{(2)}_{\mu\nu} + \mathcal{L}_{\tilde{\xi}_{(2)}} g_{\mu\nu} + \tilde{H}_{\mu\nu}, \tag{130b}$$

where

$$\tilde{H}_{\mu\nu} \coloneqq \mathcal{L}_{\tilde{\xi}_{(1)}} \left(h^{(1)}_{\mu\nu} + \frac{1}{2} \mathcal{L}_{\tilde{\xi}_{(1)}} g_{\mu\nu} \right). \tag{131}$$

Analogously, referring to the transformation rule (38), we construct invariant stress-energy perturbations,

$$\tilde{T}^{(1)}_{\mu\nu} = T^{(1)}_{\mu\nu}, \tag{132a}$$

$$\tilde{T}^{(2)}_{\mu\nu} = T^{(2)}_{\mu\nu} + \mathcal{L}_{\tilde{\xi}_{(1)}} T^{(1)}_{\mu\nu}. \tag{132b}$$

The most obvious examples of such invariants are the variables used by MP, which use the RWZ gauge conditions to specify $\tilde{h}^{(1)}_{\mu\nu}$. We review those RWZ-based invariant variables in Sec. V D below.

To our knowledge, this procedure has always specified the fixed gauge through conditions on $\tilde{h}^{(n)}_{\mu\nu}$, which then determines $\tilde{\xi}^\mu_{(1)} = \tilde{\xi}^\mu_{(1)}[h^{(1)}]$ and $\tilde{\xi}^\mu_{(2)} = \tilde{\xi}^\mu_{(2)}[h^{(1)}, h^{(2)}]$ via Eq. (130). If $h^{(n)}_{\mu\nu}$ happens to already be in the fixed gauge, then $\tilde{\xi}^\mu_{(n)} = 0$ and $\tilde{h}^{(n)}_{\mu\nu} = h^{(n)}_{\mu\nu}$. But if $h^{(n)}_{\mu\nu}$ is in any other gauge, then the quantities $\tilde{h}^{(n)}_{\mu\nu}$ are invariants constructed from $h^{(n)}_{\mu\nu}$; no matter the choice of gauge used to calculate $h^{(n)}_{\mu\nu}$, $\tilde{h}^{(n)}_{\mu\nu}$ take the value of the perturbations in the fixed gauge.

However, such a procedure is necessarily incomplete because conditions on the metric perturbation cannot fully specify the gauge. This is because of the Killing symmetries of the background. If $\xi^\mu_{(1)}$ is a Killing vector of the background, then the gauge transformation $\Delta h^{(1)}_{\mu\nu} = \mathcal{L}_{\xi_{(1)}} g_{\mu\nu}$ vanishes. This means any gauge condition on $\tilde{h}^{(1)}_{\mu\nu}$ can only fix the gauge up to infinitesimal isometries of the background.

In linear perturbation theory, this incomplete gauge fixing is not problematic. Since the ℓm modes decouple from each other, one can fully fix the $\ell > 1$ gauge freedom through conditions on the $\ell > 1$ pieces of $\tilde{h}^{(1)}_{\mu\nu}$. The gauge ambiguity is then confined to the $\ell = 0$ and $\ell = 1$ perturbations. Those perturbations are very often simply ignored because in vacuum they are only perturbations toward another stationary black hole solution (specifically, a linear-in-spin Kerr solution).

However, at second order the residual gauge ambiguity does manifest itself in the metric perturbation. If $\xi^\mu_{(1)}$ is a Killing vector of the background, then it induces a nontrivial transformation $\Delta h^{(2)}_{\mu\nu} = \mathcal{L}_{\xi_{(1)}} h^{(1)}_{\mu\nu}$. This implies that if $\tilde{\xi}^\mu_{(1)}$ is only determined up to the addition of a background Killing vector, then $\tilde{h}^{(2)}_{\mu\nu}$ is not invariant.

Appendix A analyzes the general transformation properties of $\tilde{\xi}^\mu_{(n)}$ and $\tilde{h}^{(n)}_{\mu\nu}$ and the implications of residual gauge freedom. In the body of the paper, we outline a specific type of gauge-fixing prescription that eliminates the residual freedom. Our prescription differs from others by enforcing a condition on $\tilde{T}^{(2)}_{\mu\nu}$; through Eq. (132), this imposes additional conditions on $\tilde{\xi}^\mu_{(1)}$. We then obtain vectors $\tilde{\xi}^\mu_{(1)} = \tilde{\xi}^\mu_{(1)}[h^{(1)}, T^{(2)}]$ and $\tilde{\xi}^\mu_{(2)} = \tilde{\xi}^\mu_{(2)}[h^{(1)}, h^{(2)}]$ and fully invariant perturbations $\tilde{h}^{(n)}_{\mu\nu}$ and $\tilde{T}^{(n)}_{\mu\nu}$. This restricts our prescription to nonvacuum perturbations. In global vacuum, without a matter distribution to refer to, fixing the residual gauge freedom would require specifying a value of time and angular position at some physically identifiable event in the perturbed spacetime.

We detail a particular gauge-fixing scheme in the remainder of this section. Our procedure for $\ell > 1$ follows tradition, while our procedure for $\ell = 0$ and $\ell = 1$ appears here for the first time.

D. Gauge fixing for $\ell > 1$

We follow MP and Brizuela *et al.* [48] by putting the $\ell > 1$ pieces of $\tilde{h}^{(n)}_{\mu\nu}$ in the RWZ gauge, setting

$$\tilde{h}^{(n)\ell m}_{\pm} = 0 = \tilde{h}^{(n)\ell m}_{a+}. \tag{133}$$

At first order, the analog of Eqs. (123b) and (123e) then implies that the vector $\tilde{\xi}^\mu_{(1)}$ has $\ell > 1$ modes given by

$$\tilde{\zeta}^{(1)\ell m}_a = -h^{(1)\ell m}_{a+} - r^2 \delta_a \tilde{Z}^{(1)\ell m}_+, \tag{134a}$$

$$\tilde{Z}^{(1)\ell m}_{\pm} = -\frac{h^{(1)\ell m}_{\pm}}{2r^2}. \tag{134b}$$

Substituting these formulas into the analogs of Eqs. (123a), (123c), and (123d), we find the nonzero $\ell > 1$ pieces of $\tilde{h}^{(1)}_{\mu\nu}$ are

$$\tilde{h}^{(1)\ell m}_{ab} \coloneqq h^{(1)\ell m}_{ab} + 2\delta_{(a}\tilde{\zeta}^{(1)\ell m}_{b)}, \tag{135a}$$

$$\tilde{h}^{(1)\ell m}_{a-} \coloneqq h^{(1)\ell m}_{a-} + r^2 \delta_a \tilde{Z}^{(1)\ell m}_-, \tag{135b}$$

$$\tilde{h}^{(1)\ell m}_{\circ} \coloneqq h^{(1)\ell m}_{\circ} + 2 r r_c \tilde{\zeta}^c_{(1)\ell m} - \ell(\ell+1) r^2 \tilde{Z}^{(1)\ell m}_+. \tag{135c}$$

These are the equivalent of MP's Eqs. (4.10), (4.11), and (5.7). The fields $\tilde{h}^{(1)\ell m}_{\cdot}$ are invariant regardless of what we do with $\ell = 0, 1$ modes.

At second order, the analogs of Eqs. (124b) and (124e) imply that the vector $\tilde{\xi}^\mu_{(2)}$ has $\ell > 1$ modes given by

$$\tilde{\zeta}^{(2)\ell m}_a = -h^{(2)\ell m}_{a+} - \tilde{H}^{\ell m}_{a+} - r^2 \delta_a \tilde{Z}^{(2)\ell m}_+, \tag{136a}$$

$$\tilde{Z}^{(2)\ell m}_{\pm} = -\frac{h^{(2)\ell m}_{\pm} + \tilde{H}^{\ell m}_{\pm}}{2r^2}, \tag{136b}$$

and the analogs of Eqs. (124a), (124c), and (124d) imply that the nonzero $\ell > 1$ modes of $\tilde{h}^{(2)}_{\mu\nu}$ are

$$\tilde{h}^{(2)\ell m}_{ab} \coloneqq h^{(2)\ell m}_{ab} + \tilde{H}^{\ell m}_{ab} + 2\delta_{(a}\tilde{\zeta}^{(2)\ell m}_{b)}, \tag{137a}$$

$$\tilde{h}^{(2)\ell m}_{a-} \coloneqq h^{(2)\ell m}_{a-} + \tilde{H}^{\ell m}_{a-} + r^2 \delta_a \tilde{Z}^{(2)\ell m}_-, \tag{137b}$$

$$\tilde{h}^{(2)\ell m}_{\circ} \coloneqq h^{(2)\ell m}_{\circ} + \tilde{H}^{\ell m}_{\circ} + 2 r r_c \tilde{\zeta}^c_{(2)\ell m} - \ell(\ell+1) r^2 \tilde{Z}^{(2)\ell m}_+. \tag{137c}$$

As per the discussion in the preceding section and Appendix A, these fields are not yet invariants. They only become invariant once we fix the $\ell = 0, 1$ modes of the first-order field $\tilde{h}^{(1)}_{\mu\nu}$.

E. Gauge fixing for $\ell = 0$

For $\ell = 0$, the only nonvanishing pieces of $h^{(n)}_{\mu\nu}$ are the scalar-harmonic modes $h^{(n)00}_{ab}$ and $h^{(n)00}_{\circ}$. Equation (130) reduces to

$$\tilde{h}^{(1)00}_{ab} = h^{(1)00}_{ab} + \tilde{\zeta}^c_{(1)00} \partial_c g_{ab} + 2\partial_{(a}\tilde{\zeta}^c_{(1)00} g_{b)c}, \tag{138a}$$

$$\tilde{h}^{(1)00}_{\circ} = h^{(1)00}_{\circ} + 2 r r_c \tilde{\zeta}^c_{(1)00} \tag{138b}$$

at first order. It reduces to the same equations at second order with the replacement $h^{(1)00}_{\cdot} \to h^{(2)00}_{\cdot} + \tilde{H}^{00}_{\cdot}$ on the right-hand side. Given this simple replacement, we only list results at first order in this and the next two sections below.

In these sections, we streamline the analysis by restricting ourselves to perturbations that are asymptotically flat at spatial infinity.[3] For the monopole mode, this implies

$$h^{(n)00}_{ab} = \frac{c^{(n)}_{ab}}{r} + \mathcal{O}(r^{-2}), \tag{139}$$

$$h^{(n)00}_{\circ} = r^2 \left[\frac{c^{(n)}_{\circ}}{r} + \mathcal{O}(r^{-2})\right] \tag{140}$$

for some t-independent constants $c^{(n)}_{ab}$ and $c^{(n)}_{\circ}$. Note that this restricts the gauge of $h^{(n)}_{\mu\nu}$ in addition to restricting the

[3]Lifting this restriction is straightforward. If perturbations are not asymptotically flat, or are in a gauge that does not manifest the asymptotic flatness, then integrals such as the one in Eq. (144) become ill defined. One can then take the Hadamard finite part of such integrals [91]. As an example, suppose an integrand of the form $\sum_{j=0}^{k+1} a_j r^{k-j} + \gamma(t,r)$, where $\gamma(t,r)$ falls off faster than $1/r$. We can define the integral as $\sum_{j=0}^{k} \frac{a_j}{k-j+1} r^{k-j+1} + a_{k+1} \ln r + \int_\infty^r f^{-1}(r')\gamma(t,r')dr'$. Any length scale in the logarithm can be absorbed into $\varrho^{(1)}(t)$.

asymptotic geometry. Moreover, we make the simplifying assumption that the gauge of $h^{(n)}_{\mu\nu}$ satisfies $c^{(n)}_{tr} = 0$.

We are not aware of any work that has constructed gauge invariants $\tilde{h}^{(n)00}_{ab}$ and $\tilde{h}^{(n)00}_{\circ}$ that are local functions of (t, r). We will instead allow one of the components to be a *nonlocal* function that takes the form of a radial integral. However, at least at first order we are able to construct a local invariant from it through differentiation.

We adopt the following gauge-fixing conditions:

$$\tilde{h}^{(n)00}_{\circ} = 0, \tag{141a}$$

$$\tilde{h}^{(n)00}_{tr} = 0, \tag{141b}$$

$$\lim_{r\to\infty} \tilde{h}^{(n)00}_{tt} = 0, \tag{141c}$$

where the limit is taken at fixed t.

Now, the trace condition (141a), with Eq. (138b), fully determines $\tilde{\xi}^r_{(1)00}$ to be

$$\tilde{\xi}^r_{(1)00} = -\frac{1}{2r} h^{(1)00}_{\circ}. \tag{142}$$

With Eq. (138), this in turn determines

$$\tilde{h}^{(1)00}_{rr} = h^{(1)00}_{rr} + \frac{M}{r^3 f^2} h^{(1)00}_{\circ} - \frac{1}{f}\partial_r\left(\frac{1}{r} h^{(1)00}_{\circ}\right). \tag{143}$$

The quantity $\tilde{h}^{(1)00}_{rr}$ is invariant even without specifying the remaining component $\tilde{\xi}^t_{(1)00}$. The quantity $\tilde{h}^{(2)00}_{rr}$ is given by the same formula with $h^{(1)00}_{\cdot} \to h^{(2)00}_{\cdot} + H^{00}_{\cdot}$, but it is not invariant until $\tilde{\xi}^t_{(1)00}$ is specified.

Next, the condition (141b), with the t-r component of Eq. (138), restricts $\tilde{\xi}^t_{(n)00}$ to be

$$\tilde{\xi}^t_{(1)00} = \varrho^{(1)}(t) + \int_{\infty}^{r} (f^{-1} h^{(1)00}_{tr} + f^{-2}\partial_t \tilde{\xi}^r_{(1)00}) dr', \tag{144}$$

where $\varrho^{(1)}$ is an arbitrary function of t.

The condition (141c), with the t–t component of Eq. (138), then implies

$$\varrho^{(1)} = \varrho^{(1)}_0 \tag{145}$$

for some constant $\varrho^{(1)}_0$. This represents a time translation; it is a timelike Killing vector of the background, which we cannot fix using conditions on $\tilde{h}^{(1)}_{\mu\nu}$. To fix this remaining freedom, we examine the transformation of the stress-energy tensor. We defer that procedure to Sec. V H.

The remaining nonzero component of $\tilde{h}^{(1)00}_{ab}$ is now a nonlocal invariant given by

$$\tilde{h}^{(1)00}_{tt} = h^{(1)00}_{tt} - \frac{2M}{r^2}\tilde{\xi}^r_{(1)00} - 2f\partial_t \tilde{\xi}^t_{(1)00}. \tag{146}$$

It is nonlocal because of the radial integral in $\tilde{\xi}^t_{(1)00}$. However, we can immediately construct a local invariant from it:

$$\varphi^{(1)} \coloneqq \partial_r\left(f^{-1}\tilde{h}^{(1)00}_{tt}\right), \tag{147}$$

or more explicitly,

$$\varphi^{(1)} = \partial_r(f^{-1}h^{(1)00}_{tt}) - 2f^{-1}\partial_t h^{(1)00}_{tr} + \partial_r\left(\frac{M}{r^3 f} h^{(1)00}_{\circ}\right) + \frac{1}{rf^2}\partial_t^2 h^{(1)00}_{\circ}. \tag{148}$$

Our local invariants $\tilde{h}^{(1)00}_{rr}$ and $\varphi^{(1)}$ are related to the quantities ψ_0 and o_0 in Ref. [92] by $\tilde{h}^{(1)00}_{rr} = 2\psi_0$ and $\varphi^{(1)} = 2f^{-1}o_0$.

At second order, the above formulas remain valid if we replace $h^{(1)00}_{\cdot}$ with $h^{(2)00}_{\cdot} + \tilde{H}^{00}_{\cdot}$. However, the invariant $\varphi^{(2)}$ is not manifestly local because $\tilde{H}^{00}_{\cdot}$ depends on the nonlocal quantity $\tilde{\xi}^t_{(1)00}$. It might be possible to express $\tilde{H}^{00}_{\cdot}$ in terms of local quantities, or to construct alternative second-order invariants that are manifestly local, but we leave this for interested readers to explore.

F. Gauge fixing for $\ell = 1$: Even parity

For even-parity $\ell = 1$ perturbations, the only nonvanishing pieces of $h^{(n)}_{\mu\nu}$ are the scalar- and vector-harmonic modes $h^{(n)1m}_{ab}$, $h^{(n)1m}_{\circ}$, and $h^{(n)1m}_{a+}$. Equation (130) reduces to

$$\tilde{h}^{(1)1m}_{ab} = h^{(1)1m}_{ab} + \tilde{\xi}^c_{(1)1m}\partial_c g_{ab} + 2\partial_{(a}\tilde{\xi}^c_{(1)1m} g_{b)c}, \tag{149a}$$

$$\tilde{h}^{(1)1m}_{a+} = h^{(1)1m}_{a+} + \tilde{\xi}^{(1)1m}_a + r^2\delta_a \tilde{Z}^{(1)1m}_+, \tag{149b}$$

$$\tilde{h}^{(1)1m}_{\circ} = h^{(1)1m}_{\circ} + 2rr_c\tilde{\xi}^c_{(1)1m} - 2r^2\tilde{Z}^{(1)1m}_+, \tag{149c}$$

at first order and to the same equations at second order with the replacement $h^{(1)1m}_{\cdot} \to h^{(2)1m}_{\cdot} + H^{1m}_{\cdot}$. Our assumption of asymptotic flatness implies

$$h^{(n)1m}_{ab} = \frac{c^{(n)m}_{ab}}{r^2} + \mathcal{O}(r^{-3}), \tag{150a}$$

$$h^{(n)1m}_{a+} = r\left[\frac{c^{(n)m}_{a+}}{r^2} + \mathcal{O}(r^{-3})\right], \tag{150b}$$

$$h^{(n)1m}_{\circ} = r^2\left[\frac{c^{(n)m}_{\circ}}{r^2} + \mathcal{O}(r^{-3})\right] \tag{150c}$$

for $r\to\infty$ at fixed t, where $c_{ab}^{(n)m}$, $c_{a+}^{(n)m}$, and $c_\circ^{(n)m}$ are constants.

A convenient set of gauge-fixing conditions is

$$\tilde{h}_{a+}^{(n)1m}=0, \tag{151a}$$

$$\tilde{h}_{\circ}^{(n)1m}=0, \tag{151b}$$

$$\lim_{r\to\infty}\left(\tilde{h}_{tt}^{(n)1m}\right)=0, \tag{151c}$$

$$\lim_{r\to\infty}\left(r\tilde{h}_{tr}^{(n)1m}\right)=0, \tag{151d}$$

$$\lim_{r\to\infty}\left(r^2\tilde{h}_{rr}^{(n)1m}\right)=0. \tag{151e}$$

The first of these determines $\tilde{\zeta}_a^{(1)1m}$ in terms of $\tilde{Z}_+^{(1)1m}$,

$$\tilde{\zeta}_a^{(1)1m}=-h_{a+}^{(1)1m}-r^2\delta_a\tilde{Z}_+^{(1)1m}, \tag{152}$$

and the second determines a radial differential equation for $\tilde{Z}_+^{(1)1m}$,

$$2r^2\partial_r\left(rf\tilde{Z}_+^{(1)1m}\right)=h_\circ^{(1)1m}-2rfh_{r+}^{(1)1m}. \tag{153}$$

The solution to this equation is

$$\tilde{Z}_+^{(1)1m}=\frac{\kappa^{(1)m}(t)}{rf}+\frac{1}{rf}\int_\infty^r\left(\frac{h_\circ^{(1)1m}}{2r'^2}-\frac{fh_{r+}^{(1)1m}}{r'}\right)dr', \tag{154}$$

where κ is an arbitrary function of t.

κ represents an asymptotic translation of the coordinate system. The condition (151c) imposes $\partial_t^2\kappa=0$, which enforces that the fixed gauge is not asymptotically accelerating. The condition (151d) imposes $\partial_t\kappa=0$; the fixed gauge is asymptotically stationary with respect to the asymptotic frame of $h_{\mu\nu}^{(n)}$. Finally, the condition (151e) imposes

$$\kappa^{(1)m}=\frac{1}{3M}\left(c_\circ^{(1)m}-2c_{r+}^{(1)m}\right). \tag{155}$$

The nonzero invariants are now

$$\tilde{h}_{tt}^{(1)1m}=h_{tt}^{(1)1m}-\frac{2M}{r^2}\tilde{\zeta}^r_{(1)1m}-2f\partial_t\tilde{\zeta}^t_{(1)1m}, \tag{156a}$$

$$\tilde{h}_{tr}^{(1)1m}=h_{tr}^{(1)1m}+f^{-1}\partial_t\tilde{\zeta}^r_{(1)1m}-f\partial_r\tilde{\zeta}^t_{(1)1m}, \tag{156b}$$

$$\tilde{h}_{rr}^{(1)1m}=h_{rr}^{(1)1m}-\frac{2M}{r^2f^2}\tilde{\zeta}^r_{(1)1m}+2f^{-1}\partial_r\tilde{\zeta}^r_{(1)1m}. \tag{156c}$$

Again these are nonlocal. They depend on a radial integral, and through $\kappa^{(1)m}$ they depend explicitly on the values $h_\cdot^{(1)1m}$ at spatial infinity. But again we can construct a set of local invariants through differentiation:

$$\varphi_{tt}^{(1)m}=\partial_r\left[r^4\partial_r\left(r^{-1}f\tilde{h}_{tt}^{(1)1m}\right)\right], \tag{157a}$$

$$\varphi_{tr}^{(1)m}=\partial_r\left(rf^2\tilde{h}_{tr}^{(1)1m}\right), \tag{157b}$$

$$\varphi_{rr}^{(1)m}=\partial_r\left(r^2f^3\tilde{h}_{rr}^{(1)1m}\right). \tag{157c}$$

Explicitly, in terms of $h_\cdot^{(1)1m}$,

$$\begin{aligned}\varphi_{tt}^{(1)m}=&\frac{1}{r^2}[Mr^2f\partial_r^2h_\circ-M(5r-12M)\partial_rh_\circ-r^4\partial_t^2\partial_rh_\circ\\&-2r^3\partial_t^2h_\circ+2Mr^2f\partial_rh_{r+}+2r^5f\partial_t^2\partial_rh_{r+}\\&+2r^3(3r-4M)\partial_t^2h_{r+}-2M(3r-8M)h_{r+}\\&-2r^5f\partial_t\partial_r^2h_{t+}+4r^3f\partial_th_{t+}-4r^4\partial_t\partial_rh_{t+}+r^5f\partial_r^2h_{tt}\\&+2r^4\partial_rh_{tt}-2r^3fh_{tt}]+\frac{4M}{r^3}(2r-5M)h_\circ,\end{aligned} \tag{158a}$$

$$\begin{aligned}\varphi_{tr}^{(1)m}=&\frac{1}{r^2}[-r^2f\partial_t\partial_rh_\circ+M\partial_th_\circ+rf(r-4M)\partial_th_{r+}\\&+r^3f^2\partial_t\partial_rh_{r+}-r^3f^2\partial_r^2h_{t+}-r^2f\partial_rh_{t+}\\&+r^3f^2\partial_rh_{tr}+rf(r+2M)h_{tr}]-\frac{2M}{r^3}(r-4M)h_{t+},\end{aligned} \tag{158b}$$

$$\begin{aligned}\varphi_{rr}^{(1)m}=&-\frac{f}{r}[r^2f\partial_r^2h_\circ-(r-3M)\partial_rh_\circ+2r^2f\partial_rh_{r+}\\&+2(r-M)h_{r+}-r^3f^2\partial_rh_{rr}-2rf(r+M)h_{rr}]\\&+\frac{2Mf}{r^2}h_\circ.\end{aligned} \tag{158c}$$

Here, for readability, we have omitted superscript "$(1)\ell m$" labels on the right-hand side.

Again, at second order we replace $h_\cdot^{(1)1m}$ with $h_\cdot^{(2)1m}+\tilde{H}_\cdot^{1m}$.

G. Gauge fixing for $\ell=1$: Odd parity

For odd-parity $\ell=1$ perturbations, the only nonvanishing piece of $h_{\mu\nu}^{(n)}$ is the vector-harmonic mode $h_{a-}^{(n)1m}$. At first order, Eq. (130) reduces to

$$\tilde{h}_{a-}^{(1)1m}=h_{a-}^{(1)1m}+r^2\delta_a\tilde{Z}_-^{(1)1m}. \tag{159}$$

Our assumption of asymptotic flatness at spatial infinity implies the falloff condition

$$h_{a-}^{(n)1m}=r\left[\frac{c_{a-}^{(n)}}{r^2}+\mathcal{O}(r^{-3})\right] \tag{160}$$

for some t-independent constants $c_{a-}^{(n)}$.

We impose conditions

$$\tilde{h}^{(n)1m}_{r-} = 0, \tag{161a}$$

$$\lim_{r\to\infty}\left(\tilde{h}^{(n)1m}_{t-}\right) = 0. \tag{161b}$$

The first implies

$$\tilde{Z}^{(1)1m}_{-} = \varpi^{(1)m}(t) - \int_{\infty}^{r}\frac{h^{(1)1m}_{r-}}{r'^2}dr', \tag{162}$$

and the second implies

$$\varpi^{(1)m} = \varpi^{(1)m}_{0} \tag{163}$$

for some constant $\varpi^{(1)m}_{0}$. This constant represents the rotational Killing vector of the background, and once again we are unable to determine it through conditions on $\tilde{h}^{(1)}_{\mu\nu}$.

The nonzero invariant component is

$$\tilde{h}^{(1)1m}_{t-} = h^{(1)1m}_{t-} + r^2\partial_t\tilde{Z}^{(1)1m}_{-}. \tag{164}$$

This is a nonlocal invariant, but we can construct a local invariant from it:

$$\varphi^{(1)m}_{-} \coloneqq \partial_r\left(r^{-2}\tilde{h}^{(1)1m}_{t-}\right). \tag{165}$$

Explicitly,

$$\varphi^{(1)m}_{-} = \partial_r(r^{-2}h^{(1)1m}_{t-}) - \partial_t(r^{-2}h^{(1)1m}_{r-}). \tag{166}$$

This local invariant is related to the quantity W_1 in Ref. [92] by $\varphi^{(1)m}_{-} = -W_1/r^4$.

At second order, we replace $h^{(1)1m}_{a-}$ with $h^{(2)1m}_{a-} + \tilde{H}^{1m}_{a-}$ in these formulas.

H. Residual Killing freedom and comments on gauge fixing

We have now fully fixed the gauge freedom at first and second order, up to the Killing vectors represented by the constants $\varrho^{(1)}_{0}$ and $\varpi^{(1)m}_{0}$ in Eqs. (144) and (162). To fix those remaining constants, we can impose conditions on the stress-energy tensor.

We decompose $\tilde{\xi}^{\mu}_{(1)}$ into the Killing and non-Killing pieces, denoting the former by $K^{\mu}_{(t)}$ (for the timelike Killing vector) and K^{μ} (for the rotational Killing vector), and denoting the latter by $\hat{\xi}^{\mu}_{(1)}$. The invariant $\tilde{T}^{(2)}_{\mu\nu}$ defined in Eq. (132b) is then

$$\tilde{T}^{(2)}_{\mu\nu} = T^{(2)}_{\mu\nu} + K^{\alpha}_{(t)}\partial_\alpha T^{(1)}_{\mu\nu} + \mathcal{L}_K T^{(1)}_{\mu\nu} + \mathcal{L}_{\hat{\xi}_{(1)}}T^{(1)}_{\mu\nu}. \tag{167}$$

Imposing conditions on $\tilde{T}^{(2)}_{\mu\nu}$ allows us to rearrange this to obtain equations for the constants in $K^{\mu}_{(t)}$ and K^{μ}.

The full list of now fully fixed invariants is (135), (143), (146), (156), and (164).

Having now completed our gauge-fixing procedure, we consider its merits relative to the obvious alternative: simply adopting a convenient gauge and solving the perturbative Einstein equations in that gauge. We first enumerate some merits of the gauge-fixing scheme.

(1) It fully elucidates and isolates the gauge-invariant degrees of freedom in the metric perturbation. By removing all gauge degrees of freedom, we have reduced the metric perturbation to the set of invariant fields $\tilde{h}^{(n)00}_{tt}$ and $\tilde{h}^{(n)00}_{rr}$ for $\ell = 0$; $\tilde{h}^{(n)1m}_{ab}$ and $\tilde{h}^{(n)1m}_{t-}$ for $\ell = 1$; and $\tilde{h}^{(n)\ell m}_{ab}$, $\tilde{h}^{(n)\ell m}_{a-}$, and $\tilde{h}^{(n)\ell m}_{\circ}$ for $\ell > 1$.

(2) Although the invariants are, in general, nonlocal functionals of the metric perturbation, the method also provides a simple recipe for deriving local invariants, at least at first order in perturbation theory. It might be possible to write the field equations entirely in terms of these local invariants (although we leave that possibility unexplored).

(3) Even if we wish to work with the gauge-dependent metric perturbations and choose some convenient gauge, it can be expedient to derive the field equations for the invariant variables. From them, field equations for the gauge-dependent metric perturbations can be obtained simply by substituting the definitions of $\tilde{h}^{(n)\ell m}_{\cdot}$ in terms of $h^{(n)\ell m}_{\cdot}$.

Contrast this with a clear disadvantage:

(1) Writing the Einstein equations in terms of the invariant metric perturbation components is equivalent to simply adopting the fixed gauge as one's working gauge. This might very well be an unfortunate choice, as it is often useful to choose a gauge that is well adapted to one's particular problem.

Note that this last point does not mean that working in a convenient gauge is always equivalent to working in some fully fixed gauge. If one works in a gauge with residual gauge freedom, such as the Lorenz gauge, then the residual freedom is eliminated through a choice of boundary conditions rather than at the level of the field equations.

In this paper, part of our motivation for presenting a gauge-fixing formalism is to remain in the tradition of MP. However, we recognize the merits of both approaches and therefore provide field equations both for invariant variables and for raw, gauge-dependent metric perturbations.

VI. MODE DECOMPOSITION OF THE FIRST- AND SECOND-ORDER EINSTEIN EQUATIONS

Having assembled the necessary tools, we now apply them to the Einstein field equations (16) and (17).

Sections VI A and VI B present the harmonic expansions of the quantities appearing in the field equations, relegating lengthy expressions to Appendixes B and D. Section VI D then summarizes the field equations in various forms, and Sec. VI E presents the mode-decomposed conservation equations that constrain the field equations. The special case of the field equations for $\ell = 0, 1$ is discussed in Appendix E.

We decompose the quantities in Eqs. (16) and (17) following the steps outlined above Eq. (125). In the body of the paper we present mode-decomposed formulas for the linear quantities $\mathcal{E}_{\mu\nu}[h]$ and $\mathcal{F}_{\mu\nu}[h]$ and the quadratic quantities $\mathcal{A}_{\mu\nu}[h]$, $\mathcal{B}_{\mu\nu}[h]$, and $\mathcal{C}_{\mu\nu}[h]$; the companion package PerturbationEquations includes also the decompositions of the field equations in the form (22) and (23).

We present our results in terms of the invariant fields $\tilde{h}^{(n)}_{\mu\nu}$. However, in PerturbationEquations we also provide the raw results, without the gauge-fixing procedure. As mentioned in the Introduction, to the best of our knowledge, this is the first time a complete mode decomposition has been presented for the second-order Einstein equations, with arbitrary first-order mode content and in an arbitrary gauge.

A. Linear curvature terms

Equation (9) expresses the linearized Ricci tensor $\delta R_{\mu\nu}[h]$ in terms of the quantities $\mathcal{E}_{\mu\nu}[h]$ and $\mathcal{F}_{\mu\nu}[h]$ defined in Eqs. (11) and (12). The $2+2$D decomposition of those quantities is given in Eqs. (B1) and (B2). Substituting the mode expansion (113), we obtain the modes $\mathcal{E}^{\ell m}_{\cdot}[h^{\ell m}_{\cdot}]$ and $\mathcal{F}^{\ell m}_{\cdot}[h^{\ell m}_{\cdot}]$. We then make the replacement $h_{\mu\nu} \to \tilde{h}_{\mu\nu}$, with $\tilde{h}^{\ell m}_{\pm} = 0 = \tilde{h}^{\ell m}_{a+}$.

The results are

$$\mathcal{E}^{\ell m}_{ab} = \Box_{\mathcal{M}^2}\tilde{h}^{\ell m}_{ab} + \frac{4M}{r^5}g_{ab}\left(2r^2\tilde{h}^{\ell m}_{\bullet} - \tilde{h}^{\ell m}_{\circ}\right) - \frac{4}{r^2}\tilde{h}^{\ell m}_{c(a}r_{b)}r^c + \frac{4}{r^4}\tilde{h}^{\ell m}_{\circ}r_a r_b - \frac{1}{r^2}\tilde{h}^{\ell m}_{ab}\left(\lambda^2_{\ell,1} + \frac{4M}{r}\right) + \frac{2}{r}r^c\delta_c\tilde{h}^{\ell m}_{ab}, \tag{168a}$$

$$\mathcal{E}^{\ell m}_{a+} = -\frac{2}{r^3}r_a\tilde{h}^{\ell m}_{\circ} + \frac{2}{r}\tilde{h}^{\ell m}_{ab}r^b, \tag{168b}$$

$$\mathcal{E}^{\ell m}_{a-} = \Box_{\mathcal{M}^2}\tilde{h}^{\ell m}_{a-} - \frac{1}{r^2}\tilde{h}^{\ell m}_{a-}\left(\lambda^2_{\ell,1} - \frac{2M}{r}\right) - \frac{4}{r^2}\tilde{h}^{\ell m}_{b-}r_a r^b, \tag{168c}$$

$$\mathcal{E}^{\ell m}_{\circ} = \Box_{\mathcal{M}^2}\tilde{h}^{\ell m}_{\circ} - \frac{\lambda^2_1}{r^2}\tilde{h}^{\ell m}_{\circ} - \frac{4M}{r}\tilde{h}^{\ell m}_{\bullet} + 2\tilde{h}^{\ell m}_{ab}r^a r^b - \frac{2}{r}r^a\delta_a\tilde{h}^{\ell m}_{\circ}, \tag{168d}$$

$$\mathcal{E}^{\ell m}_{\pm} = \frac{4}{r}r^a\tilde{h}^{\ell m}_{a\pm}, \tag{168e}$$

where

$$\Box_{\mathcal{M}^2} := g^{ab}\delta_a\delta_b, \tag{169}$$

and

$$\mathcal{F}^{\ell m}_{ab} = -2\delta_{(a}\delta^c\tilde{h}^{\ell m}_{b)c} + 2\delta_a\delta_b\tilde{h}^{\ell m}_{\bullet} + \frac{2}{r^2}\delta_a\delta_b\tilde{h}^{\ell m}_{\circ} - \frac{4}{r}r^c\delta_{(a}\tilde{h}^{\ell m}_{b)c} - \frac{2}{r^3}r_{(a}\delta_{b)}\tilde{h}^{\ell m}_{\circ} - \frac{4M}{r^3}\tilde{h}^{\ell m}_{ab} + \frac{4}{r^2}r^c r_{(a}\tilde{h}^{\ell m}_{b)c}, \tag{170a}$$

$$\mathcal{F}^{\ell m}_{a+} = -\delta^b\tilde{h}^{\ell m}_{ab} + 2\delta_a\tilde{h}^{\ell m}_{\bullet} + \frac{1}{r^2}\delta_a\tilde{h}^{\ell m}_{\circ} - \frac{2}{r}r_a\tilde{h}^{\ell m}_{\bullet} - \frac{2}{r}r^b\tilde{h}^{\ell m}_{ab}, \tag{170b}$$

$$\mathcal{F}^{\ell m}_{a-} = -\delta_a\delta^b\tilde{h}^{\ell m}_{b-} + \frac{2}{r}r_a\delta^b\tilde{h}^{\ell m}_{b-} - \frac{2}{r}r^b\delta_a\tilde{h}^{\ell m}_{b-} - \frac{2M}{r^3}\tilde{h}^{\ell m}_{a-} + \frac{6}{r^2}r_a r^b\tilde{h}^{\ell m}_{b-}, \tag{170c}$$

$$\mathcal{F}^{\ell m}_{\circ} = -2rr^a\delta^b\tilde{h}^{\ell m}_{ab} + 2rr^a\delta_a\tilde{h}^{\ell m}_{\bullet} - 4\tilde{h}^{\ell m}_{ab}r^a r^b - \lambda^2_{\ell,1}\tilde{h}^{\ell m}_{\bullet} + \frac{2}{r}r^a\delta_a\tilde{h}^{\ell m}_{\circ}, \tag{170d}$$

$$\mathcal{F}^{\ell m}_{+} = 2\tilde{h}^{\ell m}_{\bullet}, \tag{170e}$$

$$\mathcal{F}^{\ell m}_{-} = -2\delta^a\tilde{h}^{\ell m}_{a-} - \frac{4}{r}r^a\tilde{h}^{\ell m}_{a-}. \tag{170f}$$

Here we have written the expressions for a generic symmetric tensor $\tilde{h}_{\mu\nu}$, which can be either $\tilde{h}^{(1)}_{\mu\nu}$ or $\tilde{h}^{(2)}_{\mu\nu}$.

At first order, these expressions are valid in all gauges since (i) they are valid in at least one gauge (the gauge in which $h^{(1)}_{\mu\nu} = \tilde{h}^{(1)}_{\mu\nu}$), and (ii) they express the invariant quantity $\delta R_{\mu\nu}[h^{(1)}]$ in terms of invariant fields. If desired, we can express these quantities in terms of $h^{(1)}_{\mu\nu}$ in any gauge by substituting the explicit expressions (135), (143), (146), (156), and (164) for $\tilde{h}^{(1)}_{\mu\nu}$ in terms of $h^{(1)}_{\mu\nu}$. Alternatively, we can solve the field equations directly for the invariant fields.

At second order, $\delta R_{\mu\nu}[h^{(2)}]$ is not invariant, and the above expressions are valid *only* in the gauge for which $h^{(2)}_{\mu\nu} = \tilde{h}^{(2)}_{\mu\nu}$. However, the second-order field equation (17), taken as a whole, *is* invariant, meaning it will remain valid in all gauges after the replacements $h^{(n)}_{\mu\nu} \to \tilde{h}^{(n)}_{\mu\nu}$ and $T^{(2)}_{\mu\nu} \to \tilde{T}^{(2)}_{\mu\nu}$.

B. Quadratic curvature terms

Equation (10) expresses the second-order Ricci tensor $\delta^2 R_{\mu\nu}[h]$ in terms of the quantities $\mathcal{A}_{\mu\nu}[h]$, $\mathcal{B}_{\mu\nu}[h]$, and $\mathcal{C}_{\mu\nu}[h]$ defined in Eqs. (13)–(15). The $2+2$D decomposition of those quantities is given in Eqs. (B3)–(B5). Substituting the mode expansion (113), and following the same steps that led to Eq. (125), for $\mathcal{A}_{\mu\nu}$ we obtain

$$\mathcal{A}^{\ell m}_{ab} = \sum_{\substack{\ell' m' \ell'' m'' \\ s'=0,1}} \lambda_{\ell',s'}\lambda_{\ell'',s'} C^{\ell m 0}_{\ell' m' s' \ell'' m'' -s'} \mathcal{A}^{\ell' m' s' \ell'' m'' -s'}_{ab}, \tag{171a}$$

$$\mathcal{A}^{\ell m}_{a\pm} = \sum_{\substack{\ell' m' \ell'' m'' \\ s'=1,2}} \frac{\lambda_{\ell',s'}\lambda_{\ell'',1-s'}}{\lambda_{\ell,1}} C^{\ell m 1}_{\ell' m' s' \ell'' m'',1-s'} \mathcal{A}^{\ell' m' s' \ell'' m'',1-s'}_{a\pm}, \tag{171b}$$

$$\mathcal{A}^{\ell m}_{\circ} = \sum_{\substack{\ell' m' \ell'' m'' \\ s'=0,1,2}} \lambda_{\ell',s'}\lambda_{\ell'',s'} C^{\ell m 0}_{\ell' m' s' \ell'' m'' -s'} \mathcal{A}^{\ell' m' s' \ell'' m'' -s'}_{\circ}, \tag{171c}$$

$$\mathcal{A}^{\ell m}_{\pm} = \sum_{\substack{\ell' m' \ell'' m'' \\ s'=1,2}} \frac{\lambda_{\ell',s'}\lambda_{\ell'',2-s'}}{\lambda_{\ell,2}} C^{\ell m 2}_{\ell' m' s' \ell'' m'',2-s'} \mathcal{A}^{\ell' m' s' \ell'' m'',2-s'}_{\pm}, \tag{171d}$$

where the quantities $\mathcal{A}^{\ell' m' s' \ell'' m'' s''}_{\cdot}$ are made up of products of $h^{(1)\ell' m'}_{\cdot}$ and $h^{(1)\ell'' m''}_{\cdot}$. We display these quantities in Eq. (D3) in terms of the invariants $\tilde{h}^{(1)}_{\mu\nu}$. If $\mathcal{A}_{\mu\nu}$ is calculated in a generic gauge in terms of $h^{(1)}_{\mu\nu}$, then $s'_{\max}$ in the above sums is increased by 1 because of the involvement of the tensor modes $h^{(1)\ell' m'}_{\pm}$ and $h^{(1)\ell'' m''}_{\pm}$; in the invariant form of the field equations, those higher-spin terms appear instead on the left-hand side of the field equations, hidden within $\tilde{h}^{(2)}_{\mu\nu}$.

Similarly, $\mathcal{B}^{\ell m}_{\cdot}$ and $\mathcal{C}^{\ell m}_{\cdot}$ are given by the sums

$$\mathcal{B}^{\ell m}_{ab} = \sum_{\substack{\ell' m' \ell'' m'' \\ s'=0,1}} \lambda_{\ell',s'}\lambda_{\ell'',s'} C^{\ell m 0}_{\ell' m' s' \ell'' m'' -s'} \mathcal{B}^{\ell' m' s' \ell'' m'' -s'}_{ab}, \tag{172a}$$

$$\mathcal{B}^{\ell m}_{a\pm} = \sum_{\substack{\ell' m' \ell'' m'' \\ s'=1,2}} \frac{\lambda_{\ell',s'}\lambda_{\ell'',1-s'}}{\lambda_{\ell,1}} C^{\ell m 1}_{\ell' m' s' \ell'' m'',1-s'} \mathcal{B}^{\ell' m' s' \ell'' m'',1-s'}_{a\pm}, \tag{172b}$$

$$\mathcal{B}^{\ell m}_{\circ} = \sum_{\substack{\ell' m' \ell'' m'' \\ s'=0,1}} \lambda_{\ell',s'}\lambda_{\ell'',s'} C^{\ell m 0}_{\ell' m' s' \ell'' m'' -s'} \mathcal{B}^{\ell' m' s' \ell'' m'' -s'}_{\circ}, \tag{172c}$$

$$\mathcal{B}^{\ell m}_{\pm} = \sum_{\substack{\ell' m' \ell'' m'' \\ s'=1,2}} \frac{\lambda_{\ell',s'}\lambda_{\ell'',2-s'}}{\lambda_{\ell,2}} C^{\ell m 2}_{\ell' m' s' \ell'' m'',2-s'} \mathcal{B}^{\ell' m' s' \ell'' m'',2-s'}_{\pm}, \tag{172d}$$

$$\mathcal{C}^{\ell m}_{ab} = \sum_{\substack{\ell' m' \ell'' m'' \\ s'=0,1}} \lambda_{\ell',s'}\lambda_{\ell'',s'} C^{\ell m 0}_{\ell' m' s' \ell'' m'' -s'} \mathcal{C}^{\ell' m' s' \ell'' m'' -s'}_{ab}, \tag{173a}$$

$$\mathcal{C}^{\ell m}_{a\pm} = \sum_{\substack{\ell' m' \ell'' m'' \\ s'=1}} \frac{\lambda_{\ell',s'}\lambda_{\ell'',1-s'}}{\lambda_{\ell,1}} C^{\ell m 1}_{\ell' m' s' \ell'' m'',1-s'} \mathcal{C}^{\ell' m' s' \ell'' m'',1-s'}_{a\pm}, \tag{173b}$$

$$\mathcal{C}^{\ell m}_{\circ} = \sum_{\substack{\ell' m' \ell'' m'' \\ s'=0,1}} \lambda_{\ell',s'}\lambda_{\ell'',s'} C^{\ell m 0}_{\ell' m' s' \ell'' m'' -s'} \mathcal{C}^{\ell' m' s' \ell'' m'' -s'}_{\circ}, \tag{173c}$$

$$\mathcal{C}^{\ell m}_{\pm} = \sum_{\substack{\ell' m' \ell'' m'' \\ s'=1,2}} \frac{\lambda_{\ell',s'}\lambda_{\ell'',2-s'}}{\lambda_{\ell,2}} C^{\ell m 2}_{\ell' m' s' \ell'' m'',2-s'} \mathcal{C}^{\ell' m' s' \ell'' m'',2-s'}_{\pm}, \tag{173d}$$

where the quantities $\mathcal{B}^{\ell' m' s' \ell'' m'' s''}_{\cdot}$ and $\mathcal{C}^{\ell' m' s' \ell'' m'' s''}_{\cdot}$ are made up of products of $h^{(1)\ell' m'}_{\cdot}$ and $h^{(1)\ell'' m''}_{\cdot}$. We display these quantities in Eqs. (D4) and (D5) in terms of the invariants $\tilde{h}^{(1)}_{\mu\nu}$. In all cases, the sums run over the restricted range of mode numbers displayed in Eq. (127).

C. Stress-energy terms

The stress-energy terms in the field equations (26) are more straightforwardly decomposed. In the first-order equation we have

$$\tilde{\mathcal{T}}^{(1)\ell m}_{\cdot} = \bar{T}^{(1)\ell m}_{\cdot}, \tag{174}$$

where $\bar{T}^{(1)\ell m}_{\cdot}$ are related to $T^{(1)\ell m}_{\cdot}$ by Eq. (116). In the second-order equation we have the harmonic modes of the invariant $\tilde{\mathcal{T}}^{(2)}_{\mu\nu} = \mathcal{T}^{(2)}_{\mu\nu} + \mathcal{L}_{\xi_{(1)}}\bar{T}^{(1)}_{\mu\nu}$. Expressed in terms of the invariants $\tilde{T}^{(n)}_{\mu\nu}$ and $\tilde{h}^{(1)}_{\mu\nu}$, this quantity reads

$$\tilde{\mathcal{T}}^{(2)}_{\mu\nu} = \tilde{T}^{(2)}_{\mu\nu} - \frac{1}{2} g_{\mu\nu} g^{\alpha\beta} \tilde{T}^{(2)}_{\alpha\beta} + \frac{1}{2}\left(g_{\mu\nu}\tilde{h}^{(1)}_{\alpha\beta} - \tilde{h}^{(1)}_{\mu\nu} g_{\alpha\beta}\right) T^{\alpha\beta}_{(1)}. \tag{175}$$

Its mode expansion is given in Eq. (D6).

D. Summary of the decomposed field equations

1. Field equations in terms of invariant variables

In summary, we can write our covariant, gauge-invariant, tensor-harmonic decomposition of the Einstein equations (16) and (17) as

$$\delta R^{\ell m}_{\cdot}[\tilde{h}^{(1)\ell m}_{\cdot}] = 8\pi \mathcal{T}^{(1)\ell m}_{\cdot}, \tag{176a}$$

$$\delta R^{\ell m}_{\cdot}[\tilde{h}^{(2)\ell m}_{\cdot}] = 8\pi \tilde{\mathcal{T}}^{(2)\ell m}_{\cdot} - \delta^2 R^{\ell m}_{\cdot}[\tilde{h}^{(1)}], \tag{176b}$$

using the shorthand introduced below Eq. (107). The mode-decomposed operator on the left-hand side is

$$\delta R^{\ell m}_{\cdot}[\tilde{h}^{(n)\ell m}_{\cdot}] = -\frac{1}{2}\left(\mathcal{E}^{\ell m}_{\cdot}[\tilde{h}^{(n)\ell m}_{\cdot}] + \mathcal{F}^{\ell m}_{\cdot}[\tilde{h}^{(n)\ell m}_{\cdot}]\right), \tag{177}$$

with $\mathcal{E}^{\ell m}_{\cdot}[\tilde{h}^{(n)\ell m}_{\cdot}]$ and $\mathcal{F}^{\ell m}_{\cdot}[\tilde{h}^{(n)\ell m}_{\cdot}]$ as given in Eqs. (168) and (170).

The stress-energy source terms on the right-hand side are given in Eqs. (174) and (D6). The quadratic source term is

$$\delta^2 R^{\ell m}_{\cdot}[\tilde{h}^{(1)}] = \frac{1}{2}(\mathcal{A}^{\ell m}_{\cdot}[\tilde{h}^{(1)}] + \mathcal{B}^{\ell m}_{\cdot}[\tilde{h}^{(1)}] + \mathcal{C}^{\ell m}_{\cdot}[\tilde{h}^{(1)}]), \tag{178}$$

where the quantities $\mathcal{A}^{\ell m}_{\cdot}$, $\mathcal{B}^{\ell m}_{\cdot}$, and $\mathcal{C}^{\ell m}_{\cdot}$ are infinite sums of products of modes of $\tilde{h}^{(1)}_{\mu\nu}$. These sums take the form (171) for all three calligraphic quantities (with differing $s'_{\rm max}$), where (i) the sums run over the range in Eq. (127), (ii) $C^{\ell ms}_{\ell' m' s' \ell'' m'' s''}$ is given in Eq. (93), and (iii) (as an example) the quadratic coupling functions $\mathcal{A}^{\ell' m' s' \ell'' m'' s''}_{\cdot}$ are given in Eq. (D3).

The even- and odd-parity sectors of these field equations decouple at each order. This is because on the left-hand side of the field equations, the even-parity terms $\delta R^{\ell m}_{ab}$, $\delta R^{\ell m}_{\circ}$, $\delta R^{\ell m}_{a+}$, and $\delta R^{\ell m}_{+}$ only depend on the even-parity perturbations $\tilde{h}^{\ell m}_{ab}$ and $\tilde{h}^{\ell m}_{\circ}$; and odd-parity terms $\delta R^{\ell m}_{a-}$ and $\delta R^{\ell m}_{-}$ only depend on the odd-parity perturbations $\tilde{h}^{\ell m}_{a-}$.

However, due to the quadratic source term, the even- and odd-parity first-order fields do become coupled in the second-order field equation (176b). The even-parity fields $\tilde{h}^{(2)\ell m}_{ab}$ and $\tilde{h}^{(2)\ell m}_{\circ}$ are sourced by "even × even" products ($\tilde{h}^{(1)\ell' m'}_{ab}$ and $\tilde{h}^{(1)\ell' m'}_{\circ}$ multiplying $\tilde{h}^{(1)\ell'' m''}_{ab}$ and $\tilde{h}^{(1)\ell'' m''}_{\circ}$) as well as by "odd × odd" products ($\tilde{h}^{(1)\ell' m'}_{a-}$ multiplying $\tilde{h}^{(1)\ell'' m''}_{a-}$). The odd-parity fields $\tilde{h}^{(2)\ell m}_{a-}$ are sourced by "even × odd" products ($\tilde{h}^{(1)\ell' m'}_{ab}$ and $\tilde{h}^{(1)\ell' m'}_{\circ}$ multiplying $\tilde{h}^{(1)\ell'' m''}_{a-}$).

Similarly, the ℓm modes decouple from one another at each order, but the first-order modes couple to one another in the second-order source. A second-order mode $\tilde{h}^{(2)\ell m}_{\cdot}$ with any given ℓ value is generically sourced by *all* first-order modes $\tilde{h}^{(1)\ell' m'}_{\cdot}$ from $\ell' = 0$ to ∞.

The modes of the trace-reversed field equations (27) can be obtained from these modes using the relations (116).

2. Field equations in a generic gauge

If we do not make the replacement $h^{(n)\ell m}_{\cdot} \to \tilde{h}^{(n)\ell m}_{\cdot}$, then we arrive at the raw field equations

$$\delta R^{\ell m}_{\cdot}[h^{(n)\ell m}_{\cdot}] = \bar{S}^{(n)\ell m}_{\cdot}, \tag{179}$$

which have all the same features as Eq. (176) but are substantially more complicated due to the nonvanishing $h^{(n)\ell m}_{a\pm}$ and $h^{(n)\ell m}_{\pm}$. The sources are

$$\bar{S}^{(1)\ell m}_{\cdot} = 8\pi \mathcal{T}^{(1)\ell m}_{\cdot} = 8\pi \bar{T}^{(1)\ell m}_{\cdot}, \tag{180a}$$

$$\bar{S}^{(2)\ell m}_{\cdot} = 8\pi \mathcal{T}^{(2)\ell m}_{\cdot} - \delta^2 R^{\ell m}_{\cdot}[h^{(1)}]. \tag{180b}$$

We can also obtain these equations by starting from Eq. (176) and substituting the expressions (135), (143), (146), (156), and (164) for $\tilde{h}^{(n)\ell m}_{\cdot}$ in terms of $h^{(n)\ell m}_{\cdot}$. Additional manipulations (involving the Bianchi identities, for example) are required to put the result in precisely the form of Eq. (179), but the equations are necessarily equivalent.

3. Field equations in the Lorenz gauge

In the Lorenz gauge, where the fields $\mathcal{F}_{\mu\nu}$ and $\mathcal{C}_{\mu\nu}$ vanish, the field equations (179) reduce to

$$\mathcal{E}^{\ell m}_{\cdot}[h^{(n)\ell m}_{\cdot}] = -2\bar{S}^{(n)\ell m}_{\cdot}, \tag{181}$$

with the same first-order source $\bar{S}^{(1)\ell m}_{\cdot} = 8\pi \bar{T}^{(1)\ell m}_{\cdot}$ and with

$$\bar{S}^{(2)\ell m}_{\cdot} = 8\pi \mathcal{T}^{(2)\ell m}_{\cdot} - \frac{1}{2}\left(\mathcal{A}^{\ell m}_{\cdot}[h^{(1)}] + \mathcal{B}^{\ell m}_{\cdot}[h^{(1)}]\right). \tag{182}$$

The Lorenz-gauge field equations (at first order) in the MP harmonic basis are described in detail in Ref. [93]. Most self-force calculations in the Lorenz gauge have instead been in the closely related Barack-Lousto-Sago harmonic basis; see Table II and Appendix F.

E. Conservation equations

Because of stress-energy conservation, the source terms $S^{(n)\ell m}_{\cdot}$ in the field equations (and therefore the field equations themselves) are not all independent. They are related by the mode decomposition of the conservation equation (34), which divides into the three equations

$$\delta^b S^{\ell m}_{ab} = \frac{1}{r^3}(\lambda^2_{\ell,1} r S^{\ell m}_{a+} + 2r_a S^{\ell m}_{\circ} - 2r^2 r^b S^{\ell m}_{ab}), \tag{183a}$$

$$\delta^b S^{\ell m}_{b+} = \frac{1}{2r^2}(\mu^2_{\ell} S^{\ell m}_{+} - 4r r^b S^{\ell m}_{b+} - 2S^{\ell m}_{\circ}), \tag{183b}$$

$$\delta^b S^{\ell m}_{b-} = \frac{1}{2r^2}(\mu^2_{\ell} S^{\ell m}_{-} - 4r r^b S^{\ell m}_{b-}). \tag{183c}$$

The quantity μ^2_{ℓ} appearing here is defined in Eq. (85).

VII. MASTER SCALARS AND METRIC RECONSTRUCTION

As an alternative to directly solving the Einstein equations, a common approach in black hole perturbation theory is to instead solve one or more scalar field equations for master scalar variables. The metric perturbation is then reconstructed from the master scalar(s).

Here we summarize the formulation of this approach at second order. We specifically describe the most common variants of the approach: the RWZ formalism and the Teukolsky formalism [94,95]. Both of these are intimately related to the Weyl scalars of the perturbed spacetime, although the RWZ formalism is less often described in those terms.

The formalisms in this section are broadly identical at first and second order, with the only difference being the source terms. We therefore omit the label n that indicates a quantity's perturbative order. However, we do emphasize some particular features that distinguish the second-order problem from the first-order one.

A. Regge-Wheeler-Zerilli formalism

For the RWZ formalism we adopt the conventions of MP and Ref. [96]. Our treatment at second order differs from that of Brizuela *et al.* [48] through our choice of master scalars and our inclusion of low ($\ell = 0, 1$) modes in $h^{(1)}_{\mu\nu}$.

1. Master functions

The RWZ formalism has two master functions, one for even-parity perturbations and one for odd-parity perturbations, each of them only defined for $\ell > 1$. We specifically adopt the Zerilli-Moncrief function $\Psi^{\ell m}_{\rm even}$ [78,97] in the even-parity sector and the Cunningham-Price-Moncrief function $\Psi^{\ell m}_{\rm odd}$ [98] in the odd-parity sector, with MP's choice of normalizations. They are closely related to the real and imaginary parts, respectively, of the linearized Weyl scalar $\delta\psi_2$ [99].

In terms of our invariant metric perturbations, these functions are

$$\Psi^{\ell m}_{\rm even} = \frac{2r}{(\lambda_{\ell,1})^2}\left[r^{-2}\tilde{h}^{\ell m}_{\circ} + \frac{2}{\Lambda_\ell}\left(r^a r^b \tilde{h}^{\ell m}_{ab} - r r^a \delta_a (r^{-2}\tilde{h}^{\ell m}_{\circ})\right)\right] \tag{184}$$

and

$$\Psi^{\ell m}_{\rm odd} = \frac{2r}{\mu_\ell^2}\epsilon^{ab}\left(\delta_a \tilde{h}^{\ell m}_{b-} - \frac{2}{r} r_a \tilde{h}^{\ell m}_{b-}\right), \tag{185}$$

with

$$\Lambda_\ell \coloneqq \mu_\ell^2 + \frac{6M}{r}. \tag{186}$$

The even-parity master function satisfies the 2D scalar wave equation

$$(\Box_{\mathcal{M}^2} - V^\ell_{\rm even})\Psi^{\ell m}_{\rm even} = S^{\ell m}_{\rm even}, \tag{187}$$

with the potential

$$V^\ell_{\rm even} = \frac{1}{\Lambda_\ell^2}\left[\frac{\mu_\ell^4}{r^2}\left(\lambda^2_{\ell,1} + \frac{6M}{r}\right) + \frac{36M^2}{r^4}\left(\mu_\ell^2 + \frac{2M}{r}\right)\right]. \tag{188}$$

The source term is constructed from the source in the Einstein equation according to

$$S^{\ell m}_{\rm even} = \frac{8}{\Lambda_\ell} r^a \tilde{S}^{\ell m}_{a+} - \frac{2}{r}\tilde{S}^{\ell m}_{+} + \frac{2}{\lambda^2_{\ell,1}\Lambda_\ell}\left\{\frac{24M}{\Lambda_\ell} r^a r^b \tilde{S}^{\ell m}_{ab} - 4r^2 r^a \delta_a \tilde{S}^{\ell m}_{\bullet} + \frac{4f}{r}\tilde{S}^{\ell m}_{\circ} + \frac{2r}{\Lambda_\ell}\left[\mu_\ell^2(\mu_\ell^2 - 2) + \frac{12M}{r}(\mu_\ell^2 - 3) + \frac{84M^2}{r^2}\right]\tilde{S}^{\ell m}_{\bullet}\right\}. \tag{189}$$

The odd-parity master function likewise satisfies a 2D scalar wave equation,

$$(\Box_{\mathcal{M}^2} - V^\ell_{\rm odd})\Psi^{\ell m}_{\rm odd} = S^{\ell m}_{\rm odd}, \tag{190}$$

with the potential

$$V^\ell_{\rm odd} = \frac{\ell(\ell+1)}{r^2} - \frac{6M}{r^3} \tag{191}$$

and a source term

$$S^{\ell m}_{\rm odd} = -\frac{4r}{\mu_\ell^2}\epsilon^{ab}\delta_a \tilde{S}^{\ell m}_{b-}. \tag{192}$$

2. Metric reconstruction

From $\Psi^{\ell m}_{\rm even}$ and $\Psi^{\ell m}_{\rm odd}$, we can reconstruct the invariants $\tilde{h}^{\ell m}_{\cdot}$ for $\ell > 1$. They are given by [96]

$$\tilde{h}^{\ell m}_{tt} = f^2 \tilde{h}^{\ell m}_{rr} + 2f\tilde{S}^{\ell m}_{+}, \tag{193a}$$

$$\tilde{h}^{\ell m}_{tr} = r\partial_t\partial_r \Psi^{\ell m}_{\rm even} + rB_\ell \partial_t \Psi^{\ell m}_{\rm even} + \frac{2r^2}{\lambda^2_{\ell,1}}\left(\tilde{S}^{\ell m}_{tr} - \frac{2r}{\Lambda_\ell f}\partial_t \tilde{S}^{\ell m}_{tt}\right), \tag{193b}$$

$$\tilde{h}^{\ell m}_{rr} = \frac{1}{4r^2 f^2}\left[\Lambda_\ell\left(\lambda^2_{\ell,1} r \Psi^{\ell m}_{\rm even} - 2\tilde{h}^{\ell m}_{\circ}\right) + 4r^3 r^a \delta_a (r^{-2}\tilde{h}^{\ell m}_{\circ})\right], \tag{193c}$$

$$\tilde{h}^{\ell m}_{a-} = \frac{1}{2}\epsilon_a{}^b \delta_b (r\Psi^{\ell m}_{\rm odd}) + \frac{2r^2}{\mu_\ell^2}\tilde{S}^{\ell m}_{a-}, \tag{193d}$$

$$\tilde{h}^{\ell m}_{\circ} = r^2 r^a \delta_a \Psi^{\ell m}_{\rm even} + r^2 A_\ell \Psi^{\ell m}_{\rm even} - \frac{4r^4}{\lambda^2_{\ell,1}\Lambda_\ell}\tilde{S}^{\ell m}_{tt}, \tag{193e}$$

where

$$A_\ell \coloneqq \frac{1}{2r\Lambda_\ell}\left[\lambda^2_{\ell,2} + \frac{6M}{r}\left(\mu_\ell^2 + \frac{4M}{r}\right)\right], \tag{194}$$

$$B_\ell \coloneqq \frac{1}{rf\Lambda_\ell}\left[\mu_\ell^2\left(1 - \frac{3M}{r}\right) - \frac{6M^2}{r^2}\right]. \tag{195}$$

As pointed out by Brizuela *et al.* [48], this metric reconstruction is problematic at large r. For a linear metric perturbation that is geometrically asymptotically flat, the quantities $\tilde{h}^{(1)}_{\mu\nu}$ blow up at large r. If the second-order source is constructed from those quantities, it is also asymptotically singular. Dealing with such a source is problematic numerically but also makes the choice of physical, retarded boundary conditions unclear. We can trace the emergence of this poor behavior starting from $\Psi^{(1)\ell m}_{\rm even}$. If the first-order source is spatially bounded and we impose retarded boundary conditions, then an outgoing mode with frequency ω behaves as $\Psi^{(1)\ell m}_{\rm even} \sim e^{-i\omega u}$ at large r. The reconstruction formula (193) then implies $\tilde{h}^{(1)\ell m}_{\circ} \sim r^2 e^{-i\omega u}$ and $\tilde{h}^{(1)\ell m}_{ab} \sim r e^{-i\omega u}$; this contrasts with the natural behavior $h^{(1)\ell m}_{\circ} \sim r e^{-i\omega u}$ and $h^{(1)\ell m}_{ab} \sim r^{-1} e^{-i\omega u}$ in a well-behaved gauge. The second-order Einstein tensor then behaves as $\delta^2 G_{\mu\nu}[\tilde{h}^{(1)}, \tilde{h}^{(1)}] \sim r^2$, and the source (189) constructed from it blows up even more rapidly.

One possible route around this is to work with alternative master variables at second order. Another route, suggested by an analysis in Ref. [100], is to work with alternative variables at *first* order (or equivalently, work with $h^{(1)}_{\mu\nu}$ in a particular, nice gauge, rather than working with $\tilde{h}^{(1)}_{\mu\nu}$). We defer further discussion of asymptotics to the Conclusion and to Ref. [101], where we will provide a thorough treatment of the problem.

B. Teukolsky formalism

For the Teukolsky formalism we follow the conventions of Ref. [21]; most equations in this section are mode-decomposed, Schwarzschild specializations of equations in that reference. Our treatment also incorporates recent work on nonvacuum metric reconstruction by Green, Hollands, and Zimmerman (GHZ) [102]. Although the overarching formalism here was detailed in our earlier Ref. [100], this is the first time (to our knowledge) that a second-order Teukolsky equation has appeared in mode-decomposed form with generic first-order mode content.

1. Master scalars

We first introduce some additional tools from Geroch, Held, and Penrose (GHP) [72]. In analogy with spin-weighted quantities, a tensor v is said to have boost weight b if it transforms as $v \to \gamma^b v$ under the boost $(l^a, n^a) \to (\gamma l^a, \gamma^{-1} n^a)$. In practice, this means v's boost weight is the number of factors of l^a appearing in it minus the number of factors of n^a appearing in it. We next define derivatives $Þ$ and $Þ'$ that act on boost-weighted tensors just as ð and ð′ act on spin-weighted ones, meaning

$$Þ v = (l^a \delta_a - b\delta_a l^a) v, \tag{196a}$$

$$Þ' v = (n^a \delta_a + b\delta_a n^a) v. \tag{196b}$$

Here and below we simplify definitions using the GHP prime operation:

$$': \; m^A \leftrightarrow m^{A*}, \qquad l^a \leftrightarrow n^a. \tag{197}$$

$Þ$ raises the boost weight by 1, while $Þ'$ lowers it by 1. They satisfy the Leibniz rule [e.g., $Þ(uv) = vÞu + uÞv$ even for u and v of differing boost weights], and Eq. (60) ensures they annihilate l^a and n^a:

$$Þ l^a = Þ' l^a = Þ n^a = Þ' n^a = 0. \tag{198}$$

They satisfy the commutation relation

$$(Þ'Þ - ÞÞ') = -\epsilon^{ab}\delta_a\delta_b - \frac{2Mb}{r^3}, \tag{199}$$

and the anticommutation relation

$$(Þ'Þ + ÞÞ') = -\Box_{\mathcal{M}^2} - 2b^2(\delta_a l^a)(\delta_b n^b) + b[2(\delta_b n^b) l^a \delta_a - 2(\delta_b l^b) n^a \delta_a + (l^a \delta_a \delta_b n^b) - (n^a \delta_a \delta_b l^b)]. \tag{200}$$

They commute with ð and ð′ and with all other background quantities on S^2:

$$Þ\Omega_{AB} = Þ'\Omega_{AB} = [Þ, D_A] = [Þ', D_A] = 0. \tag{201}$$

In the Kinnersley basis in retarded coordinates (u, r), $Þ = \partial_r$ when acting on a scalar; in the Hartle-Hawking basis in advanced coordinates (v, r), $Þ' = -\partial_r$ when acting on a scalar.

The field variable in this formalism can be the linear perturbation of either of the Weyl scalars ψ_0 or ψ_4,

$$\delta\psi_0[h] \coloneqq \delta C_{\alpha\mu\beta\nu}[h] l^\alpha m^\mu l^\beta m^\nu, \tag{202a}$$

$$\delta\psi_4[h] \coloneqq \delta C_{\alpha\mu\beta\nu}[h] n^\alpha m^{\mu*} n^\beta m^{\nu*}, \tag{202b}$$

where $\delta C_{\alpha\mu\beta\nu}[h]$ is the linearized Weyl tensor. These variables are related by the GHP prime operation $\delta\psi_4 = \delta\psi_0'$. At first order, they are the first-order perturbations of the Weyl scalars, $\psi^{(1)}_0 = \delta\psi_0[h^{(1)}]$ and $\psi^{(1)}_4 = \delta\psi_4[h^{(1)}]$. However, at second order they form only part of the second-order perturbations of the Weyl scalars,

$$\psi^{(2)}_0 = \delta\psi_0[h^{(2)}] + \delta^2\psi_0[h^{(1)}, e_{(1)}], \tag{203a}$$

$$\psi^{(2)}_4 = \delta\psi_4[h^{(2)}] + \delta^2\psi_4[h^{(1)}, e_{(1)}]. \tag{203b}$$

Here $e^\alpha_{(1)}$ represents the first-order perturbations of the tetrad legs, $\{l^\alpha_{(1)}, n^\alpha_{(1)}, m^\alpha_{(1)}, m^{\alpha*}_{(1)}\}$. The quantities $\delta^2\psi_0$ and

$\delta^2\psi_4$ are quadratic in the tetrad perturbations and in $h^{(1)}_{\alpha\beta}$. In Ref. [100], we discuss some of the merits of working with $\delta\psi_0[h^{(2)}]$ or $\delta\psi_4[h^{(2)}]$ rather than with $\psi_0^{(2)}$ or $\psi_4^{(2)}$.

For easy reference in the following sections, it will be convenient to write the four-dimensional Teukolsky equations prior to mode decomposition. Written in compact form, they read

$$\hat{O}\delta\psi_0 = \hat{S}^{\alpha\beta}S_{\alpha\beta}, \tag{204a}$$

$$\hat{O}'\delta\psi_4 = \hat{S}'^{\alpha\beta}S_{\alpha\beta}, \tag{204b}$$

where we use a hat to denote linear differential operators, $S_{\alpha\beta}$ is the source in the Einstein equation $\delta G_{\alpha\beta}[h] = S_{\alpha\beta}$, and we again use the GHP prime to show the manifest symmetry between the two equations. The operators $\hat{O}$ and $\hat{S}^{\alpha\beta}$ are given explicitly in four-dimensional form in Eqs. (58) and (59) of Ref. [21] (with the conversions in Table III and $\tau = \tau' = 0$ in Schwarzschild). When acting on $\delta\psi_0$ and $\delta\psi_4$, respectively, these reduce in the Schwarzschild case to

$$\hat{O} = (Þ - 5\rho)(Þ' - \rho') - \frac{1}{2r^2}ðð' + \frac{3M}{r^3}, \tag{205a}$$

$$\hat{O}' = (Þ' - 5\rho')(Þ - \rho) - \frac{1}{2r^2}ð'ð + \frac{3M}{r^3}, \tag{205b}$$

where we have introduced

$$\rho = -\frac{r_a l^a}{r} \quad \text{and} \quad \rho' = -\frac{r_a n^a}{r}. \tag{206}$$

We will also refer to their adjoints, $\hat{O}^\dagger$ and $\hat{S}^\dagger_{\alpha\beta}$ and their GHP primes, adopting Wald's definition

$$\int A\hat{U}BdV = \int(\hat{U}^\dagger A)BdV \tag{207}$$

for any linear differential operator $\hat{U}$ and tensor test fields A and B of appropriate ranks. The operator $\hat{O}^\dagger$ is related to $\hat{O}'$ by

$$\hat{O}^\dagger = r^4\hat{O}'r^{-4}, \tag{208}$$

and $\hat{S}^\dagger_{\alpha\beta}$ is given explicitly in Eq. (60) of Ref. [21] (again with the conversions in Table III and $\tau = \tau' = 0$).

Expanded in spin-weighted harmonics, $\delta\psi_0$ and $\delta\psi_4$ read

$$\delta\psi_0 = \sum_{\ell m}\delta\psi_0^{\ell m}{}_2Y_{\ell m}, \tag{209a}$$

$$\delta\psi_4 = \sum_{\ell m}\delta\psi_4^{\ell m}{}_{-2}Y_{\ell m}, \tag{209b}$$

with coefficients

$$\delta\psi_0^{\ell m} = -\frac{1}{4r^2}\Big[\lambda_{\ell,2}h_{ll}^{\ell m} + 2^{3/2}\mu_\ell r(Þ - \rho)h_{lm}^{\ell m} + 2r^2(Þ - \rho)^2h_{mm}^{\ell m}\Big] \tag{210}$$

and

$$\delta\psi_4^{\ell m} = -\frac{1}{4r^2}\Big[\lambda_{\ell,2}h_{nn}^{\ell m} - 2^{3/2}\mu_\ell r(Þ' - \rho')h_{nm^*}^{\ell m} + 2r^2(Þ' - \rho')^2h_{m^*m^*}^{\ell m}\Big]. \tag{211}$$

Note that the formulas for $\delta\psi_0^{\ell m}$ and $\delta\psi_4^{\ell m}$ differ only by an application of the GHP prime operation and a change in sign of the term proportional to μ_ℓ; the latter change stems from the sign difference between Eqs. (88b) and (88c). This pattern carries over to the equations for the source modes below.

At the level of these ℓm modes, the Teukolsky equations (204) become

$$\left[(Þ - 5\rho)(Þ' - \rho') + \frac{\mu_\ell^2}{2r^2} + \frac{3M}{r^3}\right]\delta\psi_0^{\ell m} = S_0^{\ell m}, \tag{212a}$$

$$\left[(Þ' - 5\rho')(Þ - \rho) + \frac{\mu_\ell^2}{2r^2} + \frac{3M}{r^3}\right]\delta\psi_4^{\ell m} = S_4^{\ell m}, \tag{212b}$$

with source terms

$$S_0^{\ell m} = -\frac{\lambda_{\ell,2}}{4r^2}S_{ll}^{\ell m} - \frac{1}{\sqrt{2}r}\mu_\ell(Þ - 3\rho)S_{lm}^{\ell m} - \frac{1}{2}(Þ - 5\rho)(Þ - \rho)S_{mm}^{\ell m}, \tag{213a}$$

$$S_4^{\ell m} = -\frac{\lambda_{\ell,2}}{4r^2}S_{nn}^{\ell m} + \frac{1}{\sqrt{2}r}\mu_\ell(Þ' - 3\rho')S_{nm^*}^{\ell m} - \frac{1}{2}(Þ' - 5\rho')(Þ' - \rho')S_{m^*m^*}^{\ell m}. \tag{213b}$$

2. Green-Hollands-Zimmerman metric reconstruction

Metric reconstruction from $\delta\psi_0$ or $\delta\psi_4$ has traditionally followed a method due to Chrzanowski, Cohen, and Kegeles [103–105], neatly explained by Wald [106]. That method was specialized to homogeneous solutions with $S_{\alpha\beta} = 0$, but it has recently been extended to generic sourced perturbations by GHZ.

The method writes the metric perturbation in a radiation gauge in terms of a Hertz potential Φ and a "corrector tensor" $x_{\alpha\beta}$. We first focus on reconstruction in the IRG, in which case the perturbation reads

$$h_{\alpha\beta}^{\rm IRG} = 2{\rm Re}\left(\hat{S}^\dagger_{\alpha\beta}\Phi_{\rm IRG}\right) + x_{\alpha\beta}^{\rm IRG}. \tag{214}$$

The traditional, source-free reconstruction method uses only the first term; the corrector tensor then corrects for the failure of that method in the presence of sources.

For convenience below, we define

$$k^{\rm IRG}_{\alpha\beta} \coloneqq 2{\rm Re}\Big(\hat{S}^{\dagger}_{\alpha\beta}\Phi_{\rm IRG}\Big). \tag{215}$$

It satisfies

$$k^{\rm IRG}_{\alpha\beta} l^{\beta} = 0 = k^{\rm IRG}_{\alpha\beta} g^{\alpha\beta}, \tag{216}$$

while $x^{\rm IRG}_{\alpha\beta}$ satisfies

$$x^{\rm IRG}_{\alpha\beta} l^{\beta} = 0 \quad \text{but } x^{\rm IRG}_{\alpha\beta} g^{\alpha\beta} \neq 0. \tag{217}$$

$x^{\rm IRG}_{\alpha\beta}$ satisfies the Einstein equation

$$\delta G_{\alpha\beta}[x^{\rm IRG}] l^{\beta} = S_{\alpha\beta} l^{\beta}, \tag{218}$$

and it is only nonzero if $S_{\alpha\beta} l^{\beta} \neq 0$. $k^{\rm IRG}_{\alpha\beta}$ then satisfies the remainder of the Einstein equation,

$$\delta G_{\alpha\beta}[k^{\rm IRG}] = S_{\alpha\beta} - \delta G_{\alpha\beta}[x^{\rm IRG}] \tag{219}$$

(implying $\delta G_{\alpha\beta}[k^{\rm IRG}] l^{\beta} = 0$). Unlike $x^{\rm IRG}_{\alpha\beta}$, $k^{\rm IRG}_{\alpha\beta}$ is nonzero so long as $\delta\psi_0$ is nonzero, even if $S_{\alpha\beta}$ vanishes. The Hertz potential itself satisfies the adjoint Teukolsky equation $\hat{O}^{\dagger}\Phi_{\rm IRG} = \eta_{\rm IRG}$, where the source $\eta_{\rm IRG}$ vanishes if $S_{\alpha\beta} = 0$, but we will not require $\eta_{\rm IRG}$ explicitly.

At the level of modes, the nonzero components of $k^{\rm IRG}_{\alpha\beta}$ are given by

$$k^{\ell m}_{nn} = -\frac{\lambda_{\ell,2}}{4r^2}(\Phi^{\ell m}_{\rm IRG} + \bar{\Phi}^{\ell m}_{\rm IRG}), \tag{220a}$$

$$k^{\ell m}_{nm^*} = \frac{\mu_\ell}{2\sqrt{2}r}(\text{Þ} + 2\rho)\Phi^{\ell m}_{\rm IRG}, \tag{220b}$$

$$k^{\ell m}_{m^*m^*} = -\frac{1}{2}(\text{Þ} - \rho)(\text{Þ} + 3\rho)\Phi^{\ell m}_{\rm IRG} \tag{220c}$$

together with

$$k^{\ell m}_{nm} = (-1)^{m+1}(k^{\ell,-m}_{nm^*})^*, \tag{221a}$$

$$k^{\ell m}_{mm} = (-1)^{m}(k^{\ell,-m}_{m^*m^*})^*. \tag{221b}$$

We suppress the IRG label on the left-hand side to avoid overcrowded notation. The modes of the Hertz potential can be found by solving the inversion relation

$$\frac{1}{4}\text{Þ}^4\bar{\Phi}^{\ell m}_{\rm IRG} = \delta\psi^{\ell m}_0. \tag{222}$$

Note that for the Hertz potential (and no other quantity) we use a bar to denote the complex conjugate; modes of Φ can be obtained from modes of $\bar{\Phi}$ using Eq. (111), which in this case implies

$$\Phi^{\ell m}_{\rm IRG} = (-1)^m(\bar{\Phi}^{\ell,-m}_{\rm IRG})^*. \tag{223}$$

Because Þ is a derivative along l^a, Eq. (222) is a fourth-order ordinary differential equation along outgoing null rays. In the Kinnersley tetrad in retarded coordinates, it reduces to $\frac{1}{4}\partial_r^4\bar{\Phi}^{\ell m}_{\rm IRG} = \delta\psi^{\ell m}_0$.

Like the Hertz potential, the corrector tensor can be obtained by solving ordinary differential equations along outgoing null rays. The Einstein equation (218) reduces to the following hierarchical sequence of differential equations for the nonzero components of $x^{\rm IRG}_{\alpha\beta}$:

$$\rho^2\text{Þ}(\rho^{-2}\text{Þ}x^{\ell m}_{mm^*}) = -S^{\ell m}_{ll}, \tag{224a}$$

$$\text{Þ}[\rho^2\text{Þ}(\rho^{-2}x^{\ell m}_{nm})] = -2S^{\ell m}_{lm} + \frac{\lambda_{\ell,1}}{\sqrt{2}r}\text{Þ}x^{\ell m}_{mm^*}, \tag{224b}$$

$$\begin{aligned}\rho^2\text{Þ}(\rho^{-1}x^{\ell m}_{nn}) = -S^{\ell m}_{ln} + \bigg[\frac{\lambda^2_{\ell,1}}{2r^2} - \frac{2M}{r^3} + 2\rho\rho' \\ - 2(\rho'\text{Þ} + \rho\text{Þ}') + \text{Þ}'\text{Þ}\bigg]x^{\ell m}_{mm^*} \\ - \frac{\lambda_{\ell,1}}{2^{3/2}r}(\text{Þ} - 3\rho)(x^{\ell m}_{nm} - x^{\ell m}_{nm^*}),\end{aligned} \tag{224c}$$

together with

$$x^{\ell m}_{nm^*} = (-1)^{m+1}(x^{\ell,-m}_{nm})^*, \tag{225}$$

again suppressing the IRG label. We again recall that $\text{Þ} = \partial_r$ in the Kinnersley tetrad in retarded coordinates.

Reconstruction in the ORG is precisely analogous. All of its formulas can be obtained from those above by applying the GHP prime together with $\mu_\ell \to -\mu_\ell$ and $\lambda_{\ell,1} \to -\lambda_{\ell,1}$, beginning with the prime of Eq. (214),

$$h^{\rm ORG}_{\alpha\beta} = 2{\rm Re}(\hat{S}'^{\dagger}_{\alpha\beta}\Phi_{\rm ORG}) + x^{\rm ORG}_{\alpha\beta}. \tag{226}$$

The primed analogs of Eqs. (222) and (224) are ordinary differential equations along ingoing null rays. In this case the differential equations simplify in the Hartle-Hawking tetrad in ingoing null coordinates, for which $\text{Þ}' = -\partial_r$.

VIII. CONCLUSION

In this paper we have attempted a comprehensive treatment of the second-order perturbative field equations in a Schwarzschild background.

With tensor spherical harmonics defined in Eqs. (99) and (100) and first- and second-order metric perturbations $h^{(1)}_{\mu\nu}$

and $h^{(2)}_{\mu\nu}$ expanded as in Eq. (113), the harmonic coefficients $h^{(n)\ell m}_{\cdot}$ satisfy the first- and second-order Einstein equations (179). Those equations apply in all gauges, but the left-hand side of the equations, as well as the source terms in the second-order field equation, will take different values depending on the choice of gauge. If we specialize to the Lorenz gauge, the field equations reduce to Eq. (181). If we adopt gauge-invariant field variables, as defined in Sec. V C, then the field equations instead reduce to Eq. (176).

As an alternative to directly solving the Einstein equations, one can solve master equations for scalar variables and then reconstruct the metric perturbation. This is described in Sec. VII A within a RWZ formalism and in Sec. VII B within a Teukolsky formalism.

Regardless of which formulation is adopted, the essential ingredient in each of the second-order field equations is a coupling formula: a formula for each mode of the second-order source as an infinite sum over products of modes of the first-order field. In previous literature, such coupling formulas were presented for the Regge-Wheeler and Zerilli equations, omitting $\ell = 0, 1$ modes from both the first- and second-order fields and restricting $\ell \geq 2$ modes to the RWZ gauge (or equivalently, adopting gauge-fixed invariant RWZ variables for $\ell \geq 2$). We have presented a number of extensions and generalizations: (i) the sources in the Einstein equations in "raw" form without any gauge fixing and with arbitrary mode content, (ii) the sources in the Einstein equations in terms of invariant fields, including invariant $\ell = 0, 1$ modes derived using a novel gauge-fixing method, (iii) the second-order RWZ sources including $\ell = 0, 1$ first-order input modes, and (iv) the source in the second-order Teukolsky equation in a convenient "reduced" form. We have also, as far as possible, attempted to cast all of these in a unified framework. Most importantly, we have created the package PerturbationEquations to work with these sources in a variety of conventions.

A crucial question in all of these formulations is how quickly, if at all, the coupling formulas converge. The answer, as analyzed in Ref. [107], is that the convergence is dictated by the smoothness of the first-order field. If the first-order field contains a singularity, then its harmonic modes decay slowly in a neighborhood of the singularity, and evaluating the sum of products in the coupling formulas becomes infeasible. This challenge is critical in the self-force context, where the convergence becomes arbitrarily slow at points arbitrarily close to the particle. This has been overcome in practice using the strategy described in Ref. [107], which requires knowledge of the four-dimensional singularity structure. More efficient strategies are likely possible.

Another important question is how well the source terms behave at large distances and near the horizon. Poor behavior there will represent an obstacle to numerical integration of the field equations and difficulties in establishing physically correct boundary conditions. This has posed a problem in most second-order calculations. As reviewed in Sec. VII A, the RWZ metric variables are not asymptotically flat, which causes poor behavior of the second-order sources in the RWZ equations. This can be ameliorated by working with modified master functions. However, even in asymptotically well-behaved gauges, such as the Lorenz gauge, practical implementations can encounter nonconvergent retarded integrals [108]. This problem has been addressed by developing post-Minkowskian and near-horizon expansions that can be used to derive physical boundary conditions in the Lorenz gauge, as described in Ref. [108] and in forthcoming work. A superior method of eliminating nonconvergent integrals, explained in Refs. [100,101], is to work with variables adapted to the physical light-cone structure of the perturbed spacetime.

Follow-up papers will detail how the second-order self-force results in Refs. [30,56–58] were obtained by combining (i) the coupling formulas derived in this paper, (ii) the two-timescale expansion of the Lorenz-gauge field equations in Ref. [109], (iii) the strategies developed in Refs. [107,108] to overcome slow convergence of the coupling formulas and nonconvergence of two-timescale retarded integrals, (iv) an extension of the "puncture scheme" in Ref. [110], and (v) the punctures in Ref. [53].

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APPENDIX A: TRANSFORMATIONS OF $\tilde{\xi}^{\alpha}_{(n)}$ AND $\tilde{h}^{(n)}_{\alpha\beta}$

In Sec. V C we discuss the construction of invariant perturbations $\tilde{h}^{(n)}_{\mu\nu}$ through a procedure of gauge fixing. These invariants depend on vector fields $\tilde{\xi}^{\alpha}_{(n)}$. Here we show how $\tilde{\xi}^{\alpha}_{(n)}$ and $\tilde{h}^{(n)}_{\mu\nu}$ transform under a gauge transformation in the case of a fully fixed gauge and in the case of an only partially fixed gauge.

1. Fully fixed gauge

First we review the derivation of the standard transformation rules for metric perturbations, as displayed in Eq. (37). Perturbations $h^{(n)}_{\mu\nu}$ are defined by an identification between the background spacetime manifold and the perturbed spacetime manifold. An identification is specified by the flow of a vector field X through the one-parameter family of spacetimes, where ϵ is the parameter; see Fig. 1 of Ref. [63] for an illustration. The nth-order metric perturbation is then the nth-order term in the Taylor expansion along this flow,

$$h^{(n)}_{\mu\nu} = \frac{1}{n!}\mathcal{L}^n_X \mathsf{g}_{\mu\nu}, \tag{A1}$$

evaluated on the background manifold. If we instead work in a gauge specified by a vector field Y, then $h^{(n)}_{\mu\nu}$ is instead $\frac{1}{n!}\mathcal{L}^n_Y \mathsf{g}_{\mu\nu}$. The two quantities differ by

$$\Delta h^{(n)}_{\mu\nu} = \frac{1}{n!}\mathcal{L}^n_Y \mathsf{g}_{\mu\nu} - \frac{1}{n!}\mathcal{L}^n_X \mathsf{g}_{\mu\nu}. \tag{A2}$$

Basic manipulations of the Lie derivatives put $\Delta h^{(n)}_{\mu\nu}$ in the form (37) with the definitions

$$\xi^\mu_{(1)} \coloneqq Y^\mu - X^\mu, \tag{A3}$$

$$\xi^\mu_{(2)} \coloneqq \frac{1}{2}[X, Y]^\mu. \tag{A4}$$

Now suppose $\tilde{h}^{(n)}_{\mu\nu}$ is the nth-order metric perturbation in a gauge specified by a vector field Z, and $h^{(n)}_{\mu\nu}$ is in the gauge specified by X. Then

$$\tilde{h}^{(n)}_{\mu\nu} = h^{(n)}_{\mu\nu} + \Delta_{X\to Z} h^{(n)}_{\mu\nu}, \tag{A5}$$

where

$$\Delta_{X\to Z} h^{(n)}_{\mu\nu} = \frac{1}{n!}\mathcal{L}^n_Z \mathsf{g}_{\mu\nu} - \frac{1}{n!}\mathcal{L}^n_X \mathsf{g}_{\mu\nu}. \tag{A6}$$

This can be written in the form (130) with definitions analogous to (A3) and (A4):

$$\tilde{\xi}^\mu_{(1)} \coloneqq Z^\mu - X^\mu, \tag{A7}$$

$$\tilde{\xi}^\mu_{(2)} \coloneqq \frac{1}{2}[X, Z]^\mu. \tag{A8}$$

If $h^{(n)}_{\mu\nu}$ is instead in a gauge specified by Y, then the vectors $\tilde{\xi}^\mu_{(n)}$ become $\tilde{\xi}^\mu_{(1)} \coloneqq Z^\mu - Y^\mu$ and $\tilde{\xi}^\mu_{(2)} \coloneqq \frac{1}{2}[Y, Z]^\mu$. Therefore, under the transformation from X to Y, they transform as

$$\Delta\tilde{\xi}^\mu_{(1)} \coloneqq (Z^\mu - Y^\mu) - (Z^\mu - X^\mu), \tag{A9}$$

$$\Delta\tilde{\xi}^\mu_{(2)} \coloneqq \frac{1}{2}[Y, Z]^\mu - \frac{1}{2}[X, Z]^\mu. \tag{A10}$$

Expressing these in terms of $\xi^\mu_{(n)}$ and $\tilde{\xi}^\mu_{(n)}$, we obtain

$$\Delta\tilde{\xi}^\mu_{(1)} = -\xi^\mu_{(1)}, \tag{A11}$$

$$\Delta\tilde{\xi}^\mu_{(2)} = -\xi^\mu_{(2)} - \frac{1}{2}[\tilde{\xi}_{(1)}, \xi_{(1)}]^\mu. \tag{A12}$$

We now show that these transformation rules for $\tilde{\xi}^\mu_{(n)}$ imply the invariance of $\tilde{h}^{(n)}_{\mu\nu}$. Referring to the definition of $\tilde{h}^{(n)}_{\mu\nu}$ in Eq. (130), we see that at first order we have

$$\Delta\tilde{h}^{(1)}_{\mu\nu} = \Delta h^{(1)}_{\mu\nu} + \mathcal{L}_{\Delta\tilde{\xi}_{(1)}} g_{\mu\nu} = \mathcal{L}_{\xi_{(1)}+\Delta\tilde{\xi}_{(1)}} g_{\mu\nu}, \tag{A13}$$

where we used $\Delta h^{(1)}_{\mu\nu} = \mathcal{L}_{\xi_{(1)}} g_{\mu\nu}$. If the gauge of $\tilde{h}^{(1)}_{\mu\nu}$ is fully fixed, then $\mathcal{L}_{\xi_{(1)}+\Delta\tilde{\xi}_{(1)}} g_{\mu\nu}$ trivially vanishes because in that case $\Delta\tilde{\xi}^\mu_{(1)} = -\xi^\mu_{(1)}$.

Again referring to the definition of $\tilde{h}^{(n)}_{\mu\nu}$ in Eq. (130), we see that at second order, the gauge transformation is

$$\Delta\tilde{h}^{(2)}_{\mu\nu} = \Delta h^{(2)}_{\mu\nu} + \mathcal{L}_{\Delta\tilde{\xi}_{(2)}} g_{\mu\nu} + \Delta\tilde{H}_{\mu\nu}, \tag{A14}$$

where

$$\Delta\tilde{H}_{\mu\nu} = \mathcal{L}_{\tilde{\xi}_{(1)}+\Delta\tilde{\xi}_{(1)}}\left(h^{(1)}_{\mu\nu} + \Delta h^{(1)}_{\mu\nu} + \frac{1}{2}\mathcal{L}_{\tilde{\xi}_{(1)}+\Delta\tilde{\xi}_{(1)}} g_{\mu\nu}\right) - \mathcal{L}_{\tilde{\xi}_{(1)}}\left(h^{(1)}_{\mu\nu} + \frac{1}{2}\mathcal{L}_{\tilde{\xi}_{(1)}} g_{\mu\nu}\right). \tag{A15}$$

This can be manipulated into the form

$$\Delta\tilde{h}^{(2)}_{\mu\nu} = \mathcal{L}_{(\xi_{(2)}+\Delta\tilde{\xi}_{(2)}+\frac{1}{2}[\tilde{\xi}_{(1)},\xi_{(1)}])} g_{\mu\nu} + \mathcal{L}_{\xi_{(1)}+\Delta\tilde{\xi}_{(1)}} \tilde{h}^{(1)}_{\mu\nu} + \frac{1}{2}\mathcal{L}^2_{\xi_{(1)}+\Delta\tilde{\xi}_{(1)}} g_{\mu\nu} + \frac{1}{2}\mathcal{L}_{[\tilde{\xi}_{(1)}-\xi_{(1)},\xi_{(1)}+\Delta\tilde{\xi}_{(1)}]} g_{\mu\nu}. \tag{A16}$$

If the gauge of $\tilde{h}^{(n)}_{\mu\nu}$ is fully fixed, then this immediately vanishes by virtue of Eqs. (A11) and (A12) for $\Delta\tilde{\xi}^\mu_{(n)}$.

2. Partially fixed gauge

In many instances, the gauge is only partially (or "mostly") fixed. The most pervasive such case, discussed in Sec. V C, is when the partially fixed gauge is specified up to transformations generated by a Killing vector of the background. The gauge of $\tilde{h}^{(n)}_{\mu\nu}$ in this scenario depends on the gauge of $h^{(n)}_{\mu\nu}$.

In the geometrical description from the previous section, the vector field Z itself now depends on the gauge of $h^{(n)}_{\mu\nu}$. We can label it Z_X in the X gauge and Z_Y in the Y gauge. A short calculation leads to the following modified versions of Eqs. (A11) and (A12):

$$\Delta\tilde{\xi}^{\mu}_{(1)} = -\xi^{\mu}_{(1)} + \eta^{\mu}_{(1)}, \tag{A17}$$

$$\Delta\tilde{\xi}^{\mu}_{(2)} = -\xi^{\mu}_{(1)} - \frac{1}{2}[\tilde{\xi}_{(1)}, \xi_{(1)}]^{\mu} + \eta^{\mu}_{(2)} + \frac{1}{2}[\xi_{(1)} - \tilde{\xi}_{(1)}, \eta_{(1)}]^{\mu}, \tag{A18}$$

where $\eta^{\mu}_{(1)} \coloneqq Z^{\mu}_{Y} - Z^{\mu}_{X}$ and $\eta^{\mu}_{(2)} \coloneqq \frac{1}{2}[Z_X, Z_Y]^{\mu}$ are the generators of the transformation from the gauge defined by Z_X to the gauge defined by Z_Y. If the gauge conditions on $\tilde{h}^{(n)}_{\mu\nu}$ specify Z up to an isometry of the background, then $\eta^{\mu}_{(1)}$ and $\eta^{\mu}_{(2)}$ must be Killing vectors of the background.

Given these results, we can now assess the transformations of $\tilde{h}^{(n)}_{\mu\nu}$ using Eqs. (A13) and (A16), which remain valid in this scenario. A trivial calculation shows

$$\Delta\tilde{h}^{(1)}_{\mu\nu} = \mathcal{L}_{\eta_{(1)}} g_{\mu\nu}, \tag{A19}$$

$$\Delta\tilde{h}^{(2)}_{\mu\nu} = \mathcal{L}_{\eta_{(2)}} g_{\mu\nu} + \mathcal{L}_{\eta_{(1)}} \tilde{h}^{(1)}_{\mu\nu} + \frac{1}{2}\mathcal{L}^{2}_{\eta_{(1)}} g_{\mu\nu}. \tag{A20}$$

This is simply the expected transformation from the Z_X gauge to the Z_Y gauge. If $\eta^{\mu}_{(n)}$ are Killing vectors of the background, then

$$\Delta\tilde{h}^{(1)}_{\mu\nu} = 0 \tag{A21}$$

because $\mathcal{L}_{\eta_{(1)}} g_{\mu\nu} = 0$. Therefore $\tilde{h}^{(1)}_{\mu\nu}$ is invariant even if the gauge fixing is only specified up to background Killing symmetries. On the other hand, Eq. (A16) reduces to

$$\Delta\tilde{h}^{(2)}_{\mu\nu} = \mathcal{L}_{\eta_{(1)}} \tilde{h}^{(1)}_{\mu\nu}. \tag{A22}$$

Here we see that $\tilde{h}^{(2)}_{\mu\nu}$ is only invariant if (i) the first-order metric perturbation possesses the same Killing symmetries as $g_{\mu\nu}$ and (ii) the gauge of $\tilde{h}^{(1)}_{\mu\nu}$ respects that symmetry.

The same considerations apply for more generic unfixed low ($\ell = 0$, 1) modes. If we fix the gauge of the $\ell > 1$ modes of $\tilde{h}^{(1)}_{\mu\nu}$ but leave the gauge of the low modes entirely unfixed, then $\eta^{\mu}_{(n)}$ are generic $\ell = 0$, 1 vector fields. More concretely, if $\tilde{\xi}^{\mu}_{(1),\ell\leq 1} = 0$, then

$$\Delta\tilde{\xi}^{\mu}_{(1)} = -\xi^{\mu}_{(1),\ell>1} = -\xi^{\mu}_{(1)} + \xi^{\mu}_{(1),\ell\leq 1}; \tag{A23}$$

that is, $\eta^{\mu}_{(1)}$ is simply the $\ell = 0$, 1 piece of $\xi^{\mu}_{(1)}$. The $\ell > 1$ modes of $\tilde{h}^{(1)}_{\mu\nu}$ are invariant because, by virtue of Eq. (A19), $\Delta\tilde{h}^{(1)}_{\mu\nu}$ is confined to $\ell = 0, 1$ modes. But the $\ell > 1$ modes of $\tilde{h}^{(2)}_{\mu\nu}$ are *not* invariant because the term $\mathcal{L}_{\eta_{(1)}}\tilde{h}^{(1)}_{\mu\nu} = \mathcal{L}_{\xi_{(1),\ell\leq 1}}\tilde{h}^{(1)}_{\mu\nu}$ in Eq. (A20) generically contributes nonzero amounts to all modes of $\Delta\tilde{h}^{(2)}_{\mu\nu}$.

APPENDIX B: DECOMPOSITION OF CURVATURE TENSORS INTO TENSORS ON $\mathcal{M}^2 \times S^2$

In this appendix we provide the $2 + 2$D decompositions of the linear and quadratic quantities appearing in the Einstein equations (16) and (17), following the decomposition procedure described in Sec. III A.

1. Linear terms

The linear quantities in Eqs. (16) and (17) are $\mathcal{E}_{\mu\nu}[h]$ and $\mathcal{F}_{\mu\nu}[h]$, defined in Eqs. (11) and (12). For a generic perturbation $h_{\mu\nu}$ with components h_{ab}, h_{aA}, and h_{AB}, the $2 + 2D$ decomposition of $\mathcal{E}_{\mu\nu}$ is

$$\mathcal{E}_{ab}[h] = \delta_c\delta^c h_{ab} + \frac{1}{r^2}D_A D^A h_{ab} + \frac{2}{r^4}h^A{}_A r_a r_b + \frac{2}{r}r^c\delta_c h_{ab} - \frac{4}{r^3}D_A h_{(a}{}^A r_{b)} - \frac{4}{r^2}h_{c(a}r_{b)}r^c + 2R[\delta]_a{}^c{}_b{}^d h_{cd} - \frac{2M}{r^5}h^A{}_A q_{ab}, \tag{B1a}$$

$$\mathcal{E}_{aA}[h] = \delta_b\delta^b h_{aA} + \frac{1}{r^2}D_B D^B h_{aA} + \frac{2}{r}r^b D_A h_{ab} - \frac{2}{r^3}r_a D_B h_A{}^B - \frac{f h_{aA} + 4h^b{}_A r_a r_b}{r^2}, \tag{B1b}$$

$$\begin{aligned}\mathcal{E}_{AB}[h] = {}& \delta_a\delta^a h_{AB} + \frac{1}{r^2}D_F D^F h_{AB} - \frac{4M h_{AB}}{r^3} + 2h_{ab}r^a r^b\Omega_{AB} + \frac{2}{r}r^a(2D_{(A}h_{B)a} - \delta_a h_{AB}) + \frac{2}{r^2}R[D]_A{}^F{}_B{}^G h_{FG} \\ & + \frac{2}{r^2}f h_{AB} - \frac{2}{r^2}f h_F{}^F\Omega_{AB} - \frac{2M}{r}h_a{}^a\Omega_{AB}.\end{aligned} \tag{B1c}$$

Recall that h_{ab}, h_{aA}, and h_{AB} are defined with indices down, and their indices are raised with g^{ab} and Ω^{AB}, such that $h^{aA} \coloneqq g^{ab}\Omega^{AB}h_{bB}$, for example.

$\mathcal{F}_{\mu\nu}$ is defined in Eq. (12). Its components are found to be

$$\mathcal{F}_{ab}[h] = \frac{2M}{r^5}\bar{h}^A{}_A g_{ab} - \frac{6}{r^4}\bar{h}^A{}_A r_a r_b - 2\delta_{(a}\delta^c h_{b)c} - \frac{4}{r} r^c \delta_{(a}\bar{h}_{b)c} + \frac{2}{r^2}(2\bar{h}_{c(a} r_{b)} r^c - \delta_{(a} D^A \bar{h}_{b)A}) - \frac{4M}{r^3}\bar{h}_{ab} + \frac{2}{r^3} r_{(a}(\delta_{b)}\bar{h}^A{}_A + 2D^A \bar{h}_{b)A}), \tag{B2a}$$

$$\mathcal{F}_{aA}[h] = -\delta_a\delta_b \bar{h}^b{}_A - \frac{2}{r}[r^b(\delta_a \bar{h}_{bA} + D_A \bar{h}_{ab}) - r_a \delta_b \bar{h}^b{}_A] - D_A \delta_b \bar{h}_a{}^b + \frac{6}{r^2}\bar{h}^b{}_A r_a r_b - \frac{1}{r^2}\delta_a D_B \bar{h}_A{}^B - \frac{1}{r^2} D_A D_B \bar{h}_a{}^B - \frac{2M}{r^3}\bar{h}_{aA} + \frac{1}{r^3} r_a(D_A \bar{h}^B{}_B + 4D_B \bar{h}_A{}^B), \tag{B2b}$$

$$\mathcal{F}_{AB}[h] = -4\bar{h}_{ab} r^a r^b \Omega_{AB} - 2r^a r \Omega_{AB}\delta_b \bar{h}_a{}^b - 2D_{(A}\delta^a \bar{h}_{B)a} + \frac{2f}{r^2}\bar{h}^F{}_F \Omega_{AB} - \frac{2}{r^2} D_{(A} D^F \bar{h}_{B)F} - \frac{2}{r} r^a (2D_{(A}\bar{h}_{B)a} + \Omega_{AB} D_F \bar{h}_a{}^F), \tag{B2c}$$

where we have opted to not explicitly express $\bar{h}_{\mu\nu}$ in terms of $h_{\mu\nu}$, and parentheses around indices indicate symmetrization.

2. Quadratic terms

The quadratic quantities in Eq. (17) are $\mathcal{A}_{\mu\nu}[h]$, $\mathcal{B}_{\mu\nu}[h]$, and $\mathcal{C}_{\mu\nu}[h]$, defined in Eqs. (13)–(15). Decomposing them in the same manner as we did the linear terms, we find for $\mathcal{A}_{\mu\nu}$,

$$\begin{aligned}\mathcal{A}_{ab}[h] = {}& 2r^{-6} h_{AB} h^{AB} r_a r_b + \frac{1}{2}\delta_a h^{cd}\delta_b h_{cd} - 2r^{-5} h^{AB} r_{(a}\delta_{b)} h_{AB} + 2\delta_{[d} h_{c]b}\delta^d h_a{}^c + 2r^{-4} D_{[B} h_{A]b} D^B h_a{}^A \\ & - 2r^{-3} h^{cA} r_{(a}(\delta_{b)} h_{cA} - \delta_{|c|} h_{b)A} + D_{|A|} h_{b)c}) + r^{-2}\delta_a h^{cA}\delta_b h_{cA} + r^{-2}\delta_c h_{bA}\delta^c h_a{}^A \\ & - 2r^{-2}\delta^c h_{(a}{}^A D_{|A|} h_{b)c} + r^{-2} D_A h_{bc} D^A h_a{}^c + 2r^{-4} h_{cA} h^{cA} r_a r_b + \frac{1}{2} r^{-4}\delta_a h^{AB}\delta_b h_{AB},\end{aligned} \tag{B3a}$$

$$\begin{aligned}\mathcal{A}_{aA}[h] = {}& -\delta_b h_{ac}\delta^c h^b{}_A + \delta_c h_{ab}\delta^c h^b{}_A + \frac{1}{2}\delta_a h^{bc} D_A h_{bc} - r^{-1} h^b{}_A r^c (2\delta_{[a} h_{b]c} + \delta_c h_{ab}) + r^{-1} h_b{}^c r^b D_A h_{ac} \\ & + r^{-1} h_{bc} r^b (\delta_a h^c{}_A - \delta^c h_{aA}) - r^{-5} h^{BF} r_a D_A h_{BF} - r^{-3} h_{AB} r^b (\delta_a h_b{}^B + \delta_b h_a{}^B) + r^{-3} h_A{}^B r^b D_B h_{ab} \\ & + 2r^{-3} h^{bB}(r_{(b}\delta_{a)} h_{AB} + D_A h_{B[a} r_{b]} - D_B h_{A(a} r_{b)}) - 2r^{-2} h^b{}_A h_{bc} r_a r^c + r^{-2}\delta_b h_{AB}\delta^b h_a{}^B + r^{-2}\delta_a h^{bB} D_A h_{bB} \\ & - r^{-2}\delta^b h_a{}^B D_B h_{bA} - r^{-2}\delta^b h_A{}^B D_B h_{ab} + r^{-2} D_B h_{ab} D^B h^b{}_A - 2r^{-4} h^{bB} h_{AB} r_a r_b + \frac{1}{2} r^{-4}\delta_a h^{BF} D_A h_{BF} \\ & + 2r^{-4} D_{[F} h_{B]A} D^F h_a{}^B,\end{aligned} \tag{B3b}$$

$$\begin{aligned}\mathcal{A}_{AB}[h] = {}& 2h_a{}^c h_{bc} r^a r^b \Omega_{AB} - \delta_a h_{bB}\delta^b h^a{}_A + \delta_b h_{aB}\delta^b h^a{}_A + r^{-1} h^a{}_B r^b (2\delta_{[a} h_{b]A} - D_A h_{ab}) + 2f r^{-4} h_A{}^F h_{BF} \\ & + 2r^{-1} r^a (2h_{ab} D_{(A} h^b{}_{B)} - h_a{}^b \delta_b h_{AB}) + r^{-1} h^a{}_A r^b (2\delta_{[a} h_{b]B} - D_B h_{ab}) + \frac{1}{2} D_A h^{ab} D_B h_{ab} - 2r^{-3} h_{(A}{}^F r^a \delta_{|a|} h_{B)F} \\ & - 2r^{-3} h_{F(A} r^a D_{B)} h_a{}^F + 4r^{-3} h^{aF} r_a D_{(A} h_{B)F} - 2r^{-3} h^{aF} r_a D_F h_{AB} + 2r^{-3} h_{F(A} r^a D^F h_{B)a} + 2f r^{-2} h_{aB} h^a{}_A \\ & + 2r^{-2} h^{aF} h^b{}_F r_a r_b \Omega_{AB} + r^{-2}\delta_a h_{BF}\delta^a h_A{}^F + r^{-2} D_A h^{aF} D_B h_{aF} - 2r^{-2}\delta_a h_{F(A} D^F h^a{}_{B)} + r^{-2} D_F h_{aB} D^F h^a{}_A \\ & + \frac{1}{2} r^{-4} D_A h^{FG} D_B h_{FG} + 2r^{-4} D_{[G} h_{F]B} D^G h_A{}^F,\end{aligned} \tag{B3c}$$

where square brackets indicate antisymmetrization and vertical bars indicate that the enclosed indices are excluded from the symmetrization or antisymmetrization. For $\mathcal{B}_{\mu\nu}$,

$$\begin{aligned}\mathcal{B}_{ab}[h] = {}& -2M r^{-7} h_{AB} h^{AB} g_{ab} + 2r^{-6} h_{AB} h^{AB} r_a r_b - 2M r^{-5} h_{cA} h^{cA} g_{ab} - 2r^{-5} h^{AB} r_{(a}\delta_{b)} h_{AB} \\ & + h^{cd}(\delta_b\delta_a h_{cd} - \delta_d\delta_a h_{bc} - \delta_d\delta_b h_{ac} + \delta_d\delta_c h_{ab}) - r^{-3} h^A{}_A r^c (2\delta_{(a} h_{b)c} - \delta_c h_{ab}) \\ & + r^{-3} h^{cA}[2r_c(2\delta_{(a} h_{b)A} - D_A h_{ab}) - 2r_{(a}(\delta_{b)} h_{cA} + \delta_{|c|} h_{b)A} - D_{|A|} h_{b)c})] + r^{-2} h^{cA}(2\delta_b\delta_a h_{cA} - 2\delta_c\delta_{(a} h_{b)A} \\ & - 2D_A\delta_{(a} h_{b)c} + 2D_A\delta_c h_{ab}) + r^{-4} h^{AB}(\delta_b\delta_a h_{AB} + D_B D_A h_{ab}) - 2r^{-4} h_{AB} D^B \delta_{(a} h_{b)}{}^A,\end{aligned} \tag{B4a}$$

$$\begin{aligned}\mathcal{B}_{aA}[h] = {}& h_{bc}(\delta^c\delta^b h_{aA} - \delta^c\delta_a h^b{}_A) + 2Mr^{-3}h^b{}_A h_{ab} + r^{-1}h^b{}_A r^c(2\delta_{(a}h_{b)c} - \delta_c h_{ab}) + r^{-3}h_{AB}r^b\delta_a h_b{}^B \\ & - r^{-1}h_{bc}[r^b(\delta_a h^c{}_A + \delta^c h_{aA}) - 2r_a\delta^c h^b{}_A] + r^{-1}h_b{}^c r^b D_A h_{ac} - r^{-1}h^{bc}r_a D_A h_{bc} + 2h^{bc}D_A\delta_{[a}h_{c]b} \\ & + 2r^{-3}h^{bB}r_{(a}\delta_{b)}h_{AB} - r^{-3}h_{AB}r^b\delta_b h_a{}^B + 6r^{-3}h^{bB}r_{[b}D_{|A|}h_{a]B} - r^{-3}h^B{}_B r^b(2\delta_{[a}h_{b]A} + D_A h_{ab}) \\ & + 6r^{-3}h^{bB}r_{[a}D_{|B|}h_{b]A} + r^{-3}h_A{}^B r^b D_B h_{ab} - r^{-2}h^{bB}(\delta_b\delta_a h_{AB} + 2\delta_b D_{[A}h_{B]a} - 2D_A\delta_a h_{bB} + 2D_B\delta_{[a}h_{b]A} \\ & + D_B D_A h_{ab}) + 2Mr^{-5}h_a{}^B h_{AB} + 4r^{-5}h^{BF}r_a D_{[F}h_{A]B} - 4r^{-4}h^{bB}h_{AB}r_a r_b + 2r^{-4}h^b{}_A h^B{}_B r_a r_b \\ & + r^{-4}h^{BF}D_A\delta_a h_{BF} - r^{-4}h^{BF}D_F\delta_a h_{AB} - r^{-4}h_{BF}D^F D_A h_a{}^B + r^{-4}h_{BF}D^F D^B h_{aA},\end{aligned}\tag{B4b}$$

$$\begin{aligned}\mathcal{B}_{AB}[h] = {}& -2h_{ab}\delta^b D_{(A}h^a{}_{B)} + 2r^{-3}h_{F(A}r^a D^F h_{B)a} + h^{bc}r^a r\Omega_{AB}(\delta_a h_{bc} - 2\delta_c h_{ab}) + h^{ab}(\delta_b\delta_a h_{AB} + D_B D_A h_{ab}) \\ & - 2Mr^{-1}h_{ab}h^{ab}\Omega_{AB} + 2r^{-1}h^a{}_A r^b\delta_{[a}h_{b]B} - 4r^{-1}h^{aF}r^b\Omega_{AB}\delta_{[a}h_{b]F} - 2r^{-1}h_a{}^b r^a\delta_b h_{AB} \\ & + r^{-1}h^a{}_B r^b(2\delta_{[a}h_{b]A} + D_A h_{ab}) + r^{-1}h^a{}_A r^b D_B h_{ab} - 2r^{-1}h^{aF}r^b\Omega_{AB}D_F h_{ab} - 4r^{-2}h^a{}_A h^b{}_B r_a r_b \\ & + 4r^{-2}h_{ab}h_{AB}r^a r^b + 4r^{-2}h^{aF}h^b{}_F r_a r_b\Omega_{AB} - 2r^{-2}h_{ab}h^F{}_F r^a r^b\Omega_{AB} + 2r^{-2}f(h_{aB}h^a{}_A - h_{aF}h^{aF}\Omega_{AB}) \\ & - 2r^{-2}h^{aF}\delta_a D_{(A}h_{B)F} - 4r^{-3}h^{aF}r_a D_F h_{AB} + r^{-2}h^{aF}\delta_a D_F h_{AB} + 2r^{-2}h^{aF}D_B D_A h_{aF} + r^{-2}h^{aF}D_F\delta_a h_{AB} \\ & - 2r^{-2}h^{aF}D_F D_{(A}h_{B)a} - 2r^{-3}h_{FG}r^a\Omega_{AB}D^G h_a{}^F + 2fr^{-4}(h_A{}^F h_{BF} - h_{FG}h^{FG}\Omega_{AB}) \\ & + r^{-4}h^{FG}(D_B D_A h_{FG} - 2D_G D_{(A}h_{B)F} + D_G D_F h_{AB}) - 2Mr^{-3}h_{aF}h^{aF}\Omega_{AB} - 2r^{-3}h_{(A}{}^F r^a\delta_{|a|}h_{B)F} \\ & + r^{-3}h^{FG}r^a\Omega_{AB}\delta_a h_{FG} + 2r^{-3}h_{F(A}r^a D_{B)}h_a{}^F + 4r^{-3}h^{aF}r_a D_{(A}h_{B)F} + r^{-3}h^F{}_F r^a(\delta_a h_{AB} - 2D_{(A}h_{B)a}).\end{aligned}\tag{B4c}$$

For $\mathcal{C}_{\mu\nu}$,

$$\begin{aligned}\mathcal{C}_{ab}[h] = {}& -2r^{-1}h_c{}^d r^c(2\delta_{(a}h_{b)d} - \delta_d h_{ab}) + \frac{1}{2}(2\delta_{(a}h_{b)}{}^c - \delta^c h_{ab})(\delta_c h^d{}_d - 2\delta_d h_c{}^d) - 2r^{-3}h^{cA}r_c(2\delta_{(a}h_{b)A} - D_A h_{ab}) \\ & + \frac{1}{2}r^{-2}[2\delta_{(a}h_{b)}{}^c\delta_c h^A{}_A - \delta_c h^A{}_A\delta^c h_{ab} - 4\delta_{(a}h_{b)c}D_A h^{cA} + 2\delta_c h_{ab}D_A h^{cA} + 2\delta_c h^{cA}D_A h_{ab} \\ & + 2\delta_{(a}h_{b)}{}^A(D_A h^c{}_c - 2\delta_c h^c{}_A) - D_A h^c{}_c D^A h_{ab}] + \frac{1}{2}r^{-4}(2\delta_{(a}h_{b)}{}^A - D^A h_{ab})(D_A h^B{}_B - 2D_B h_A{}^B),\end{aligned}\tag{B5a}$$

$$\begin{aligned}\mathcal{C}_{aA}[h] = {}& -r^{-1}r_a h^b{}_A(\delta_b h^c{}_c - 2\delta_c h_b{}^c) - 2r^{-1}r^b h_{bc}(\delta_a h^c{}_A - \delta^c h_{aA}) - r^{-5}h_A{}^B r_a(D_B h^F{}_F - 2D_F h_B{}^F) \\ & - 2r^{-1}r^b h_b{}^c D_A h_{ac} + \frac{1}{2}[\delta_a h^b{}_A(\delta_b h^c{}_c - 2\delta_c h_b{}^c) - \delta_b h^c{}_c\delta^b h_{aA} + 2\delta^b h_{aA}\delta_c h_b{}^c - 2\delta_b h^{bc}D_A h_{ac} \\ & + \delta^c h^b{}_b D_A h_{ac}] - 2r^{-3}h^{bB}r_b(\delta_a h_{AB} + 2D_{[A}h_{B]a}) + r^{-3}r_a[2h_{AB}\delta_b h^{bB} - h^b{}_A(\delta_b h^B{}_B - 2D_B h_b{}^B) - h_A{}^B D_B h^b{}_b] \\ & + \frac{1}{2}r^{-2}[8h^b{}_A h_{bc}r_a r^c - 2\delta_a h_{AB}\delta_b h^{bB} + \delta_a h^b{}_A\delta_b h^B{}_B - \delta_b h^B{}_B\delta^b h_{aA} - 2\delta_b h^{bB}D_A h_{aB} + \delta^b h^B{}_B D_A h_{ab} \\ & + 2\delta_b h^{bB}D_B h_{aA} - 2\delta_a h^b{}_A D_B h_b{}^B + 2\delta^b h_{aA}D_B h_b{}^B - 2D_A h_{ab}D_B h^{bB} + \delta_a h_A{}^B D_B h^b{}_b + D_A h_a{}^B D_B h^b{}_b \\ & - D_B h^b{}_b D^B h_{aA}] + 4r^{-4}h^{bB}h_{AB}r_a r_b + \frac{1}{2}r^{-4}(\delta_a h_A{}^B + D_A h_a{}^B - D^B h_{aA})(D_B h^F{}_F - 2D_F h_B{}^F),\end{aligned}\tag{B5b}$$

$$\begin{aligned}\mathcal{C}_{AB}[h] = {}& h_a{}^b r^a r\Omega_{AB}(\delta_b h^c{}_c - 2\delta_c h_b{}^c) + \frac{1}{2}(2\delta_a h^{ab}\delta_b h_{AB} - 8h_a{}^c h_{bc}r^a r^b\Omega_{AB} - \delta_b h_{AB}\delta^b h^a{}_a + 2\delta_a h^b{}_b D_{(A}h^a{}_{B)} \\ & - 4\delta_b h_a{}^b D_{(A}h^a{}_{B)}) + r^{-1}r^a[h_a{}^b(2\delta_b h_{AB} + \Omega_{AB}\delta_b h^F{}_F) - 2h_{ab}(2D_{(A}h^b{}_{B)} + \Omega_{AB}D_F h^{bF})] \\ & + r^{-1}h^{aF}r_a\Omega_{AB}(D_F h^b{}_b - 2\delta_b h^b{}_F) + \frac{1}{2}r^{-4}(2D_{(A}h_{B)}{}^F - D^F h_{AB})(D_F h^G{}_G - 2D_G h_F{}^G) \\ & - \frac{1}{2}r^{-2}[8h^{aF}h^b{}_F r_a r_b\Omega_{AB} + 4\delta_a h^{aF}D_{(A}h_{B)F} - \delta_a h^F{}_F(2D_{(A}h^a{}_{B)} - \delta^a h_{AB}) + 4D_{(A}h^a{}_{B)}D_F h_a{}^F \\ & - 2\delta_a h_{AB}D_F h^{aF} - 2\delta_a h^{aF}D_F h_{AB} - 2D_{(A}h_{B)F}D^F h^a{}_a + D_F h_{AB}D^F h^a{}_a] \\ & + r^{-3}r_a h^{aF}(2D_F h_{AB} - 4D_{(A}h_{B)F} + \Omega_{AB}D_F h^G{}_G - 2\Omega_{AB}D_G h_F{}^G).\end{aligned}\tag{B5c}$$

APPENDIX C: COVARIANT DERIVATIVES OF SCALAR HARMONICS

Our method of decomposing the Einstein equation requires expressing covariant derivatives of $Y_{\ell m}$ in terms of spin-weighted harmonics. We do so by noting that each covariant derivative in $D_{A_1}\cdots D_{A_s}Y_{\ell m}$ acts on a tensor of spin weight 0, such that Eqs. (79a) and (79b) imply $D_A = \frac{1}{2}(\tilde{m}_A\eth' + \tilde{m}^*_A\eth)$. Using this along with Eq. (80), we find

$$D_{A_1}\cdots D_{A_s}Y_{\ell m} = \frac{1}{2^s}(\tilde{m}_{A_1}\eth' + \tilde{m}^*_{A_1}\eth)\cdots(\tilde{m}_{A_s}\eth' + \tilde{m}^*_{A_s}\eth)Y_{\ell m} \tag{C1a}$$

$$= \frac{1}{2^s}\sum_{\sigma(s)}\prod_{j=1}^{s}\alpha^s_{i,j}(\tilde{m}_{A_j}\eth')Y_{\ell m} \tag{C1b}$$

$$= \frac{1}{2^s}[\tilde{m}_{A_1}\cdots\tilde{m}_{A_s}\eth'^s Y_{\ell m} + \tilde{m}^*_{A_1}\cdots\tilde{m}^*_{A_s}\eth^s Y_{\ell m} + \cdots]. \tag{C1c}$$

The sum runs over all of the 2^s distinct products of $\tilde{m}_{A_j}\eth'$ and $\tilde{m}^*_{A_j}\eth$ (with s total factors) acting on $Y_{\ell m}$. This is made precise in the second line, where $\sigma(s)$ is the set of s-tuples with all elements either 0 or 1, $\sigma(s)_{i,j}$ is the jth element of the ith s-tuple, $\alpha^s_{i,j}(\tilde{m}_{A_j}\eth') = \tilde{m}_{A_j}\eth'$ if $\sigma(s)_{i,j} = 0$, and $\alpha^s_{i,j}(\tilde{m}_{A_j}\eth') = \tilde{m}^*_{A_j}\eth$ if $\sigma(s)_{i,j} = 1$.

This sum is straightforwardly written in terms of spin-weighted harmonics using the definition (83) and the identities (88). For $s = 1$ and $s = 2$, the results are Eqs. (90) and (91). For $s = 3$ and $s = 4$, the results are

$$D_A D_B D_C Y_{\ell m} = \frac{1}{8}\lambda_{\ell,3}({}_{-3}Y_{\ell m}\tilde{m}_A\tilde{m}_B\tilde{m}_C - {}_3Y_{\ell m}\tilde{m}^*_A\tilde{m}^*_B\tilde{m}^*_C) + \frac{1}{8}\lambda_{\ell,2}\sqrt{(l+2)(l-1)}({}_1Y_{\ell m}\tilde{m}_A\tilde{m}^*_B\tilde{m}^*_C - {}_{-1}Y_{\ell m}\tilde{m}^*_A\tilde{m}_B\tilde{m}_C)$$
$$- \frac{1}{4}\lambda^3_{\ell,1}({}_{-1}Y_{\ell m}\tilde{m}_A - {}_1Y_{\ell m}\tilde{m}^*_A)\Omega_{BC}, \tag{C2}$$

and

$$D_A D_B D_C D_D Y_{\ell m} = \frac{1}{16}\lambda_{\ell,4}({}_{-4}Y_{\ell m}\tilde{m}_A\tilde{m}_B\tilde{m}_C\tilde{m}_D + {}_4Y_{\ell m}\tilde{m}^*_A\tilde{m}^*_B\tilde{m}^*_C\tilde{m}^*_D) - \frac{1}{16}\lambda_{\ell,2}\{{}_2Y_{\ell m}[(l+3)(l-2)\tilde{m}_A\tilde{m}^*_B$$
$$+ (l+2)(l-1)\tilde{m}^*_A\tilde{m}_B]\tilde{m}^*_C\tilde{m}^*_D + {}_{-2}Y_{\ell m}[(l+3)(l-2)\tilde{m}^*_A\tilde{m}_B + (l+2)(l-1)\tilde{m}_A\tilde{m}^*_B]\tilde{m}_C\tilde{m}_D\}$$
$$- \frac{1}{8}\lambda^3_{\ell,1}\sqrt{(l+2)(l-1)}({}_{-2}Y_{\ell m}\tilde{m}_A\tilde{m}_B + {}_2Y_{\ell m}\tilde{m}^*_A\tilde{m}^*_B)\Omega_{CD} + \frac{1}{4}\lambda^4_{\ell,1}\Omega_{AB}\Omega_{CD}Y_{\ell m}$$
$$+ \frac{1}{16}\lambda^2_{\ell,2}(\tilde{m}_A\tilde{m}_B\tilde{m}^*_C\tilde{m}^*_D + \tilde{m}^*_A\tilde{m}^*_B\tilde{m}_C\tilde{m}_D)Y_{\ell m}. \tag{C3}$$

Equation (C1) can also be used to derive the relationships (98) between tensor and spin-weighted harmonics. $Y^{\ell m}_{A_1\cdots A_s}$ is the symmetric trace-free piece of Eq. (C1), which picks out the two terms that contain only $\tilde{m}$'s or only $\tilde{m}^*$'s. Equation (98a) then immediately follows from the definition (83). Given the identity (71), the definition (97) of $X^{\ell m}_{A_1\cdots A_s}$ likewise picks out the two terms that contain only $\tilde{m}$'s or only $\tilde{m}^*$'s in Eq. (C1), and Eq. (98b) then immediately follows.

APPENDIX D: QUADRATIC COUPLING FUNCTIONS

In this appendix we list the coupling functions appearing in the decompositions of quadratic quantities. We only provide expressions for even-parity coupling functions: for example, $\mathcal{A}^{\ell' m' s' \ell'' m'' s''}_{a+}$ and $\mathcal{A}^{\ell' m' s' \ell'' m'' s''}_{+}$. Odd-parity analogs can be obtained using the rule

$$\begin{aligned}\mathcal{A}^{\ell' m' s' \ell'' m'' s''}_{a-} &= -i\mathcal{A}^{\ell' m' s' \ell'' m'' s''}_{a+}\\ \mathcal{A}^{\ell' m' s' \ell'' m'' s''}_{-} &= -i\mathcal{A}^{\ell' m' s' \ell'' m'' s''}_{+}\end{aligned} \quad \text{with} \quad \sigma_\pm \to -\sigma_\mp. \tag{D1}$$

The quantities $\sigma \coloneqq (-1)^{\ell+\ell'+\ell''}$ and $\sigma_\pm \coloneqq \sigma \pm 1$ arise from use of Eq. (94).

1. Gauge transformation

The coupling functions appearing in Eq. (125) are

$$H_{ab}^{\ell'm'0\ell''m''0} = 2h_{c(a}^{\ell''m''}\delta_{b)}\zeta_{\ell'm'}^{c} + \zeta_{\ell''m''}^{c}\delta_c h_{ab}^{\ell'm'} + \delta_{(a}\zeta_{\ell'm'}^{c}\delta_{b)}\zeta_c^{\ell''m''} + \zeta_{\ell''m''}^{c}\delta_c\delta_{(a}\zeta_{b)}^{\ell'm'} + \delta_{(a}\zeta_{|c|}^{\ell'm'}\delta^c\zeta_{b)}^{\ell''m''}, \tag{D2a}$$

$$\begin{aligned}
H_{ab}^{\ell'm'1\ell''m''-1} = &-\frac{i}{2}\Big[h_{ab}^{\ell''m''}(Z_{\ell'm'}^{-} - iZ_{\ell'm'}^{+}) - h_{ab}^{\ell'm'}(Z_{\ell''m''}^{-} + iZ_{\ell''m''}^{+}) + 2(h_{(a+}^{\ell''m''} - ih_{(a-}^{\ell''m''})(\delta_{b)}Z_{\ell'm'}^{-} - i\delta_{b)}Z_{\ell'm'}^{+}) \\
&- 2(h_{(a+}^{\ell'm'} + ih_{(a-}^{\ell'm'})(\delta_{b)}Z_{\ell''m''}^{-} + i\delta_{b)}Z_{\ell''m''}^{+})\Big] + r^2(\delta_{(a}Z_{\ell''m''}^{-} + i\delta_{(a}Z_{\ell''m''}^{+})(i\delta_{b)}Z_{\ell'm'}^{+} - \delta_{b)}Z_{\ell'm'}^{-}) \\
&- \frac{i}{2}\Big[\zeta_{(a}^{\ell''m''}(\delta_{b)}Z_{\ell'm'}^{-} - i\delta_{b)}Z_{\ell'm'}^{+}) - \zeta_{(a}^{\ell'm'}(\delta_{b)}Z_{\ell''m''}^{-} + i\delta_{b)}Z_{\ell''m''}^{+}) - (Z_{\ell''m''}^{-} + iZ_{\ell''m''}^{+})\delta_{(a}\zeta_{b)}^{\ell'm'} \\
&+ (Z_{\ell'm'}^{-} - iZ_{\ell'm'}^{+})\delta_{(a}\zeta_{b)}^{\ell''m''}\Big],
\end{aligned} \tag{D2b}$$

$$\begin{aligned}
H_{a+}^{\ell'm'1\ell''m''0} = &\frac{1}{4}\Big\{2\sigma_+ h_{ac}^{\ell''m''}\zeta_{\ell'm'}^{c} + \lambda_{\ell'',1}^{2}\Big[i\sigma_- h_{a+}^{\ell''m''}Z_{\ell'm'}^{-} - \sigma_+ h_{a-}^{\ell'm'}Z_{\ell''m''}^{-} - i\sigma_- h_{a+}^{\ell'm'}Z_{\ell''m''}^{-} - \sigma_+ h_{a+}^{\ell''m''}Z_{\ell'm'}^{+} \\
&+ h_{a-}^{\ell''m''}(\sigma_+ Z_{\ell'm'}^{-} + i\sigma_- Z_{\ell'm'}^{+}) + i\sigma_- h_{a-}^{\ell'm'}Z_{\ell''m''}^{+} - \sigma_+ h_{a+}^{\ell'm'}Z_{\ell''m''}^{+}\Big] - 2i\sigma_- h_{\circ}^{\ell''m''}\delta_a Z_{\ell'm'}^{-} \\
&+ 2\sigma_+ h_{\circ}^{\ell''m''}\delta_a Z_{\ell'm'}^{+} - 2i\sigma_- h_{c-}^{\ell'm'}\delta_a\zeta_{\ell''m''}^{c} + 2\sigma_+ h_{c+}^{\ell'm'}\delta_a\zeta_{\ell''m''}^{c} - 2i\sigma_-\zeta_{\ell''m''}^{c}\delta_c h_{a-}^{\ell'm'} + 2\sigma_+\zeta_{\ell''m''}^{c}\delta_c h_{a+}^{\ell'm'}\Big\} \\
&- rr_c\zeta_{\ell''m''}^{c}(i\sigma_-\delta_a Z_{\ell'm'}^{-} - \sigma_+\delta_a Z_{\ell'm'}^{+}) + \frac{1}{8}\Big[\lambda_{\ell'',1}^{2}(-i\sigma_- Z_{\ell''m''}^{-}\zeta_a^{\ell'm'} - \sigma_+ Z_{\ell''m''}^{+}\zeta_a^{\ell'm'} + i\sigma_- Z_{\ell'm'}^{-}\zeta_a^{\ell''m''} \\
&- \sigma_+ Z_{\ell'm'}^{+}\zeta_a^{\ell''m''}) + 2\sigma_+\zeta_{\ell'm'}^{c}\delta_a\zeta_c^{\ell''m''} + 2\sigma_+\zeta_{\ell'm'}^{c}\delta_a\zeta_c^{\ell''m''} + 2\sigma_+\zeta_{\ell''m''}^{c}\delta_c\zeta_a^{\ell'm'} + 2\sigma_+\zeta_{\ell'm'}^{c}\delta_c\zeta_a^{\ell''m''}\Big] \\
&+ \frac{1}{8}r^2\Big\{-Z_{\ell''m''}^{-}\lambda_{\ell'',1}^{2}(\sigma_+\delta_a Z_{\ell'm'}^{-} + i\sigma_-\delta_a Z_{\ell'm'}^{+}) + 3Z_{\ell''m''}^{+}\lambda_{\ell'',1}^{2}(i\sigma_-\delta_a Z_{\ell'm'}^{-} - \sigma_+\delta_a Z_{\ell'm'}^{+}) \\
&+ \lambda_{\ell'',1}^{2}[(\sigma_+ Z_{\ell'm'}^{-} + i\sigma_- Z_{\ell'm'}^{+})\delta_a Z_{\ell''m''}^{-} + (i\sigma_- Z_{\ell'm'}^{-} - \sigma_+ Z_{\ell'm'}^{+})\delta_a Z_{\ell''m''}^{+}] + 2\sigma_+\zeta_{\ell''m''}^{c}\delta_c\delta_a Z_{\ell'm'}^{+} \\
&- 2i\sigma_-\delta_a(\zeta_{\ell''m''}^{c}\delta_c Z_{\ell'm'}^{-}) + 2\sigma_+\delta_a\zeta_{\ell''m''}^{c}\delta_c Z_{\ell'm'}^{+}\Big\},
\end{aligned} \tag{D2c}$$

$$\begin{aligned}
H_{a+}^{\ell'm'2\ell''m''-1} = &-\frac{1}{4}h_{a-}^{\ell''m''}(\sigma_+ Z_{\ell'm'}^{-} + i\sigma_- Z_{\ell'm'}^{+}) + \frac{i}{4}\Big[h_{a+}^{\ell''m''}(\sigma_- Z_{\ell'm'}^{-} + i\sigma_+ Z_{\ell'm'}^{+}) - \sigma_- h_{a+}^{\ell'm'}Z_{\ell''m''}^{-} + i\sigma_+ h_{a+}^{\ell'm'}Z_{\ell''m''}^{+} \\
&+ h_{a-}^{\ell'm'}(i\sigma_+ Z_{\ell''m''}^{-} + \sigma_- Z_{\ell''m''}^{+}) + i\sigma_+ h_{-}^{\ell'm'}\delta_a Z_{\ell''m''}^{-} - \sigma_- h_{+}^{\ell'm'}\delta_a Z_{\ell''m''}^{-} + (\sigma_- h_{-}^{\ell'm'} + i\sigma_+ h_{+}^{\ell'm'})\delta_a Z_{\ell''m''}^{+}\Big] \\
&- \frac{1}{8}\Big[(i\sigma_- Z_{\ell''m''}^{-} + \sigma_+ Z_{\ell''m''}^{+})\zeta_a^{\ell'm'} - (i\sigma_- Z_{\ell'm'}^{-} - \sigma_+ Z_{\ell'm'}^{+})\zeta_a^{\ell''m''}\Big] \\
&- \frac{1}{8}r^2\Big[3(\sigma_+ Z_{\ell'm'}^{-} + i\sigma_- Z_{\ell'm'}^{+})\delta_a Z_{\ell''m''}^{-} + Z_{\ell''m''}^{-}(\sigma_+\delta_a Z_{\ell'm'}^{-} + i\sigma_-\delta_a Z_{\ell'm'}^{+}) \\
&- Z_{\ell''m''}^{+}(i\sigma_-\delta_a Z_{\ell'm'}^{-} - \sigma_+\delta_a Z_{\ell'm'}^{+}) - 3i(\sigma_- Z_{\ell'm'}^{-} + i\sigma_+ Z_{\ell'm'}^{+})\delta_a Z_{\ell''m''}^{+}\Big],
\end{aligned} \tag{D2d}$$

$$\begin{aligned}
H_{\circ}^{\ell'm'0\ell''m''0} = &-h_{\circ}^{\ell''m''}Z_{\ell'm'}^{+}\lambda_{\ell',1}^{2} + \zeta_{\ell''m''}^{c}\delta_c h_{\circ}^{\ell'm'} + r_a r_c\zeta_{\ell'm'}^{c}\zeta_{\ell''m''}^{a} + \frac{M}{r}\zeta_c^{\ell'm'}\zeta_{\ell''m''}^{c} - r_c r(2Z_{\ell'm'}^{+}\zeta_{\ell''m''}^{c}\lambda_{\ell',1}^{2} \\
&- \zeta_{\ell''m''}^{a}\delta_a\zeta_{\ell'm'}^{c}) + \frac{1}{2}r^2\lambda_{\ell',1}^{2}(Z_{\ell'm'}^{+}Z_{\ell''m''}^{+}\lambda_{\ell'',1}^{2} - \zeta_{\ell''m''}^{c}\delta_c Z_{\ell'm'}^{+}),
\end{aligned} \tag{D2e}$$

$$H_{\circ}^{\ell'm'1\ell''m''-1} = \frac{i}{2}\left[h_{\circ}^{\ell''m''}(iZ^{+}_{\ell'm'} - Z^{-}_{\ell'm'}) + h_{\circ}^{\ell'm'}(Z^{-}_{\ell''m''} + iZ^{+}_{\ell''m''}) + (h_{c-}^{\ell''m''} + ih_{c+}^{\ell''m''})\zeta^{c}_{\ell'm'} - (h_{c-}^{\ell'm'} - ih_{c+}^{\ell'm'})\zeta^{c}_{\ell''m''}\right.$$
$$-\frac{1}{2}\zeta^{c}_{\ell'm'}\zeta^{\ell''m''}_{c} + \frac{i}{2}r_c r[(Z^{-}_{\ell''m''} + iZ^{+}_{\ell''m''})\zeta^{c}_{\ell'm'} - (Z^{-}_{\ell'm'} - iZ^{+}_{\ell'm'})\zeta^{c}_{\ell''m''}]$$
$$+\frac{1}{4}r^2\Big\{-iZ^{-}_{\ell''m''}Z^{+}_{\ell'm'}\lambda^2_{\ell',1} + Z^{+}_{\ell''m''}[iZ^{-}_{\ell'm'}\lambda^2_{\ell'',1} + Z^{+}_{\ell'm'}(\lambda^2_{\ell',1} + \lambda^2_{\ell'',1})]$$
$$\left.-\zeta^{c}_{\ell''m''}(i\delta_c Z^{-}_{\ell'm'} + \delta_c Z^{+}_{\ell'm'}) + i\zeta^{c}_{\ell'm'}(\delta_c Z^{-}_{\ell''m''} + i\delta_c Z^{+}_{\ell''m''})\Big\}, \tag{D2f}$$

$$H_{\circ}^{\ell'm'2\ell''m''-2} = \frac{1}{4}\left[(h_{-}^{\ell''m''} + ih_{+}^{\ell''m''})(Z^{-}_{\ell'm'} - iZ^{+}_{\ell'm'}) + (h_{-}^{\ell'm'} - ih_{+}^{\ell'm'})(Z^{-}_{\ell''m''} + iZ^{+}_{\ell''m''})\right]$$
$$+\frac{1}{2}r^2(Z^{-}_{\ell'm'} - iZ^{+}_{\ell'm'})(Z^{-}_{\ell''m''} + iZ^{+}_{\ell''m''}), \tag{D2g}$$

$$H_{+}^{\ell'm'1\ell''m''1} = \frac{1}{4}\mu^2_{\ell'}[(\sigma_+ h_{-}^{\ell'm'} + i\sigma_- h_{+}^{\ell'm'})Z^{-}_{\ell''m''} + (i\sigma_- h_{-}^{\ell'm'} - \sigma_+ h_{+}^{\ell'm'})Z^{+}_{\ell''m''}] - (i\sigma_- h_{c-}^{\ell''m''} - \sigma_+ h_{c+}^{\ell''m''})\zeta^{c}_{\ell'm'}$$
$$+\frac{1}{2}\sigma_+\zeta^{c}_{\ell'm'}\zeta^{\ell''m''}_{c} + \frac{1}{4}r^2\Big\{\mu^2_{\ell'}[Z^{-}_{\ell'm'}(\sigma_+ Z^{-}_{\ell''m''} + i\sigma_- Z^{+}_{\ell''m''}) + Z^{+}_{\ell'm'}(i\sigma_- Z^{-}_{\ell''m''} - \sigma_+ Z^{+}{}_{\ell''m''})]$$
$$-2\zeta^{c}_{\ell'm'}(i\sigma_-\delta_c Z^{-}_{\ell''m''} - \sigma_+\delta_c Z^{+}_{\ell''m''})\Big\}, \tag{D2h}$$

$$H_{+}^{\ell'm'2\ell''m''0} = -\frac{i}{2}\left[2h_{\circ}^{\ell''m''}(\sigma_- Z^{-}_{\ell'm'} + i\sigma_+ Z^{+}_{\ell'm'}) + \sigma_- h_{+}^{\ell'm'}Z^{-}_{\ell''m''}\lambda^2_{\ell'',1} - i\sigma_+ h_{+}^{\ell'm'}Z^{+}_{\ell''m''}\lambda^2_{\ell'',1}\right.$$
$$\left.-h_{-}^{\ell'm'}(i\sigma_+ Z^{-}_{\ell''m''} + \sigma_- Z^{+}_{\ell''m''})\lambda^2_{\ell'',1} + \sigma_-\zeta^{c}_{\ell''m''}\delta_c h_{-}^{\ell'm'} + i\sigma_+\zeta^{c}_{\ell''m''}\delta_c h_{+}^{\ell'm'}\right]$$
$$-2r_c r(i\sigma_- Z^{-}_{\ell'm'} - \sigma_+ Z^{+}_{\ell'm'})\zeta^{c}_{\ell''m''} - \frac{1}{2}r^2\left[i\sigma_- Z^{-}_{\ell''m''}Z^{+}_{\ell'm'}\lambda^2_{\ell'',1} + 2\sigma_+ Z^{+}_{\ell'm'}Z^{+}_{\ell''m''}\lambda^2_{\ell'',1}\right.$$
$$\left.+Z^{-}_{\ell'm'}(\sigma_+ Z^{-}_{\ell''m''} - 2i\sigma_- Z^{+}_{\ell''m''})\lambda^2_{\ell'',1} + i\sigma_-\zeta^{c}_{\ell''m''}\delta_c Z^{-}_{\ell'm'} - \sigma_+\zeta^{c}_{\ell''m''}\delta_c Z^{+}_{\ell'm'}\right], \tag{D2i}$$

$$H_{+}^{\ell'm'3\ell''m''-1} = -\frac{1}{4}[(\sigma_+ h_{-}^{\ell'm'} + i\sigma_- h_{+}^{\ell'm'})Z^{-}_{\ell''m''} - (i\sigma_- h_{-}^{\ell'm'} - \sigma_+ h_{+}^{\ell'm'})Z^{+}_{\ell''m''}] - \frac{1}{4}r^2[Z^{-}_{\ell''m''}(\sigma_+ Z^{-}_{\ell'm'} + i\sigma_- Z^{+}_{\ell'm'})$$
$$-(i\sigma_- Z^{-}_{\ell'm'} - \sigma_+ Z^{+}_{\ell'm'})Z^{+}_{\ell''m''}]. \tag{D2j}$$

2. Ricci tensor

The quantities appearing in Eq. (171) are

$$\mathcal{A}_{ab}^{\ell'm'0\ell''m''0} = \frac{4\tilde{h}_{\circ}^{\ell'm'}\tilde{h}_{\circ}^{\ell''m''}r_a r_b}{r^6} + \frac{1}{2}\delta_a\tilde{h}_{cd}^{\ell'm'}\delta_b\tilde{h}_{ef}^{\ell''m''}g^{ce}g^{df} - \frac{4\tilde{h}_{\circ}^{\ell''m''}r_{(a}\delta_{b)}\tilde{h}_{\circ}^{\ell'm'}}{r^5} + \frac{\tilde{h}_{b-}^{\ell'm'}\tilde{h}_{a-}^{\ell''m''}\lambda^2_{\ell',1}\lambda^2_{\ell'',1}}{r^4} + \frac{\delta_a\tilde{h}_{\circ}^{\ell'm'}\delta_b\tilde{h}_{\circ}^{\ell''m''}}{r^4}$$
$$+2\delta_{[d}\tilde{h}_{c]b}^{\ell'm'}\delta^d\tilde{h}_{ae}^{\ell''m''}g^{ce}, \tag{D3a}$$

$$\mathcal{A}_{ab}^{\ell'm'1\ell''m''-1} = -\frac{2\tilde{h}_{c-}^{\ell'm'}\tilde{h}_{d-}^{\ell''m''}g^{cd}r_a r_b}{r^4} - \frac{r_{(a}g^{cd}(i\tilde{h}_{b)c}^{\ell'm'} - \delta_{b)}\tilde{h}_{c-}^{\ell'm'} + \delta_{|c|}\tilde{h}_{b)-}^{\ell'm'})\tilde{h}_{d-}^{\ell''m''}}{r^3}$$
$$+\frac{r_{(a}g^{cd}(i\tilde{h}_{b)c}^{\ell''m''} + \delta_{b)}\tilde{h}_{c-}^{\ell''m''} - \delta_{|c|}\tilde{h}_{b)-}^{\ell''m''})\tilde{h}_{d-}^{\ell'm'}}{r^3} - \frac{g^{cd}(\tilde{h}_{c(a}^{\ell'm'}\tilde{h}_{b)d}^{\ell''m''} + \delta_{(a}\tilde{h}_{|c|-}^{\ell''m''}\delta_{b)}\tilde{h}_{d-}^{\ell'm'})}{r^2}$$
$$-\frac{\delta_c\tilde{h}_{(a-}^{\ell'm'}\delta^c\tilde{h}_{b)-}^{\ell''m''} - i(\tilde{h}_{c(a}^{\ell''m''}\delta^c\tilde{h}_{b)-}^{\ell'm'} - \tilde{h}_{c(a}^{\ell'm'}\delta^c\tilde{h}_{b)-}^{\ell''m''})}{r^2}, \tag{D3b}$$

$$\begin{aligned}\mathcal{A}_{a+}^{\ell'm'1\ell''m''0} = &-\frac{\sigma_+\tilde{h}_\circ^{\ell'm'}\tilde{h}_\circ^{\ell''m''}r_a}{r^5} + \frac{i\sigma_-\tilde{h}_{b-}^{\ell'm'}\tilde{h}_\circ^{\ell''m''}r_a r^b}{r^4} + \frac{1}{2r^4}\tilde{h}_\circ{}^{\ell'm'}(i\sigma_-\tilde{h}_{a-}^{\ell''m''}\lambda^2_{\ell'',1} + \sigma_+\delta_a\tilde{h}_\circ^{\ell''m''})\\ &-\frac{1}{2r^3}\tilde{h}_{b-}^{\ell'm'}r^b(\sigma_+\tilde{h}_{a-}^{\ell''m''}\lambda^2_{1,\ell''} + i\sigma_-\delta_a\tilde{h}_\circ{}^{\ell''m''}) + \frac{1}{2r^3}\tilde{h}_\circ^{\ell''m''}r^b(\sigma_+\tilde{h}_{ab}^{\ell'm'} + 2i\sigma_-\delta_{(a}\tilde{h}_{b)-}^{\ell'm'})\\ &-\frac{1}{2r^3}i\sigma_-\tilde{h}_{b-}^{\ell'm'}r_a\delta^b\tilde{h}_\circ^{\ell''m''} + \frac{1}{r^2}i\sigma_-\tilde{h}_{bc}^{\ell''m''}\tilde{h}_{d-}^{\ell'm'}r_a g^{bd}r^c - \frac{1}{2r^2}\sigma_+\tilde{h}_{b-}^{\ell''m''}\lambda^2_{\ell'',1}g^{bc}\delta_{(a}\tilde{h}_{c)-}^{\ell'm'}\\ &-\frac{1}{4r^2}\left[2i\sigma_-\delta_b\tilde{h}_\circ^{\ell''m''}\delta^b\tilde{h}_{a-}^{\ell'm'} - \tilde{h}_{ab}^{\ell'm'}g^{bc}\left(i\sigma_-\tilde{h}_{c-}^{\ell''m''}\lambda^2_{\ell'',1} - 2\sigma_+\delta_c\tilde{h}_\circ^{\ell''m''}\right)\right]\\ &+\frac{1}{2r}i\sigma_-\tilde{h}_{b-}^{\ell'm'}g^{bd}r^c\left(\delta_a\tilde{h}_{cd}^{\ell''m''} - 2\delta_{[d}\tilde{h}_{c]a}^{\ell''m''}\right) + \frac{1}{2r}\tilde{h}_{bc}^{\ell''m''}r^b g^{cd}\left(\sigma_+\tilde{h}_{ad}^{\ell'm'} - 2i\sigma_-\delta_{[a}\tilde{h}_{d]-}^{\ell'm'}\right)\\ &+\frac{1}{4}g^{bd}(\sigma_+\tilde{h}_{bc}^{\ell'm'}\delta_a\tilde{h}_{de}^{\ell''m''}g^{ce} + 4i\sigma_-\delta_{[b}\tilde{h}_{c]a}^{\ell''m''}\delta^c\tilde{h}_{d-}^{\ell'm'}),\end{aligned} \tag{D3c}$$

$$\mathcal{A}_{a+}^{\ell'm'2\ell''m''-1} = \frac{\sigma_+\tilde{h}_{b-}^{\ell'm'b}\tilde{h}_{c-}^{\ell''m''}g^{bc}r_a}{2r^3} + \frac{\tilde{h}_{b-}^{\ell'm'}g^{bc}(i\sigma_-\tilde{h}_{ac}^{\ell''m''} + 2\sigma_+\delta_{[c}\tilde{h}_{a]-}^{\ell''m''})}{4r^2}, \tag{D3d}$$

$$\begin{aligned}\mathcal{A}_\circ^{\ell'm'0\ell''m''0} = &2\tilde{h}_{ad}^{\ell'm'}\tilde{h}_{bc}^{\ell''m''}g^{cd}r^a r^b + \frac{2f\tilde{h}_\circ^{\ell'm'}\tilde{h}_\circ^{\ell''m''}}{r^4} - \frac{2\tilde{h}_\circ^{\ell''m''}r^a\delta_a\tilde{h}_\circ^{\ell'm'}}{r^3} + \frac{\tilde{h}_{a-}^{\ell'm'}\tilde{h}_{b-}^{\ell''m''}g^{ab}\lambda^2_{\ell',1}\lambda^2_{\ell'',1}}{2r^2}\\ &+\frac{\delta_a\tilde{h}_\circ^{\ell''m''}\delta^a\tilde{h}_\circ^{\ell'm'}}{r^2} - \frac{2\tilde{h}_{ab}^{\ell''m''}r^a\delta^b\tilde{h}_\circ^{\ell'm'}}{r},\end{aligned} \tag{D3e}$$

$$\begin{aligned}\mathcal{A}_\circ^{\ell'm'1\ell''m''-1} = &-\frac{\tilde{h}_\circ^{\ell'm'}\tilde{h}_\circ^{\ell''m''}}{r^4} - \frac{(fg^{ab} + 2r^a r^b)\tilde{h}_{a-}^{\ell'm'}\tilde{h}_{b-}^{\ell''m''}}{r^2} - \frac{i}{2r}r^b g^{ac}\tilde{h}_{c-}^{\ell''m''}\left(\tilde{h}_{ab}^{\ell'm'} - 2i\delta_{[a}\tilde{h}_{b]-}^{\ell'm'}\right)\\ &+\frac{i}{2r}r^b g^{ac}\tilde{h}_{c-}^{\ell'm'}\left(\tilde{h}_{ab}^{\ell''m''} + 2i\delta_{[a}\tilde{h}_{b]-}^{\ell''m''}\right) - \frac{1}{4}g^{ac}\left(\tilde{h}_{ab}^{\ell'm'}\tilde{h}_{cd}^{\ell''m''}g^{bd} - 4\delta_{[a}\tilde{h}_{b]-}^{\ell''m''}\delta^b\tilde{h}_{c-}^{\ell'm'}\right),\end{aligned} \tag{D3f}$$

$$\mathcal{A}_\circ^{\ell'm'2\ell''m''-2} = \frac{g^{ab}\tilde{h}_{a-}^{\ell'm'}\tilde{h}_{b-}^{\ell''m''}}{2r^2}, \tag{D3g}$$

$$\begin{aligned}\mathcal{A}_+^{\ell'm'1\ell''m''1} = &-\frac{2i\sigma_-\tilde{h}_{a-}^{\ell''m''}\tilde{h}_\circ^{\ell'm'}r^a}{r^3} - \frac{\sigma_+ f\tilde{h}_{a-}^{\ell'm'}\tilde{h}_{b-}^{\ell''m''}g^{ab}}{r^2} + \frac{\tilde{h}_{a-}^{\ell''m''}g^{ac}r^b(i\sigma_-\tilde{h}_{bc}^{\ell'm'} + 2\sigma_+\delta_{[b}\tilde{h}_{c]-}^{\ell'm'})}{r}\\ &+\frac{1}{4}\sigma_+ g^{ac}(\tilde{h}_{ab}^{\ell'm'}\tilde{h}_{cd}^{\ell''m''}g^{bd} + 4\delta_{[a}\tilde{h}_{b]-}^{\ell''m''}\delta^b\tilde{h}_{c-}^{\ell'm'}),\end{aligned} \tag{D3h}$$

$$\mathcal{A}_+^{\ell'm'2\ell''m''0} = -\frac{2i\sigma_-\tilde{h}_{ab}^{\ell''m''}\tilde{h}_{c-}^{\ell'm'}r^b g^{ac}}{r} + \frac{i\sigma_-\tilde{h}_{a-}^{\ell'm'}\delta^a\tilde{h}_\circ^{\ell''m''}}{r^2}. \tag{D3i}$$

The quantities appearing in Eq. (172) are

$$\begin{aligned}\mathcal{B}_{ab}^{\ell'm'0\ell''m''0} = &\frac{4(rr_a r_b - Mg_{ab})\tilde{h}_\circ^{\ell'm'}\tilde{h}_\circ^{\ell''m''}}{r^7} - \frac{4\tilde{h}_\circ^{\ell''m''}r_{(a}\delta_{b)}\tilde{h}_\circ^{\ell'm'}}{r^5} + \frac{\tilde{h}_\circ^{\ell''m''}(2\delta_a\delta_b\tilde{h}_\circ^{\ell'm'} - \lambda^2_{\ell',1}\tilde{h}_{ab}^{\ell'm'})}{r^4}\\ &-\frac{2\tilde{h}_\circ^{\ell''m''}r^c(2\delta_{(a}\tilde{h}_{b)c}^{\ell'm'} - \delta_c\tilde{h}_{ab}^{\ell'm'})}{r^3} + \tilde{h}_{ef}^{\ell''m''}g^{ce}g^{df}(\delta_b\delta_a\tilde{h}_{cd}^{\ell'm'} + \delta_d\delta_c\tilde{h}_{ab}^{\ell'm'} - 2\delta_d\delta_{(a}\tilde{h}_{b)c}^{\ell'm'}),\end{aligned} \tag{D4a}$$

$$\mathcal{B}_{ab}^{\ell'm'1\ell''m''-1} = \frac{2Mg^{cd}\tilde{h}_{c-}^{\ell'm'}\tilde{h}_{d-}^{\ell''m''}g_{ab}}{r^5} - \frac{r^c[\tilde{h}_{c-}^{\ell'm'}(2\delta_{(a}\tilde{h}_{b)-}^{\ell''m''} - i\tilde{h}_{ab}^{\ell''m''}) + \tilde{h}_{c-}^{\ell''m''}(2\delta_{(a}\tilde{h}_{b)-}^{\ell'm'} + i\tilde{h}_{ab}^{\ell'm'})]}{r^3}$$
$$+ \frac{g^{cd}r_{(a}[(\delta_{b)}\tilde{h}_{d-}^{\ell'm'} + \delta_{|d|}\tilde{h}_{b)-}^{\ell'm'} + i\tilde{h}_{b)d}^{\ell'm'})\tilde{h}_{c-}^{\ell''m''} + (\delta_{b)}\tilde{h}_{d-}^{\ell''m''} + \delta_{|d|}\tilde{h}_{b)-}^{\ell''m''} - i\tilde{h}_{b)d}^{\ell''m''})\tilde{h}_{c-}^{\ell'm'}]}{r^3}$$
$$+ \frac{g^{cd}\tilde{h}_{c-}^{\ell''m''}[2\delta_d\delta_{(a}\tilde{h}_{b)-}^{\ell'm'} - 2\delta_b\delta_a\tilde{h}_{d-}^{\ell'm'} + 2i(\delta_d\tilde{h}_{ab}^{\ell'm'} - \delta_{(a}\tilde{h}_{b)d}^{\ell'm'})]}{2r^2}$$
$$+ \frac{g^{cd}\tilde{h}_{c-}^{\ell'm'}[2\delta_d\delta_{(a}\tilde{h}_{b)-}^{\ell''m''} - 2\delta_b\delta_a\tilde{h}_{d-}^{\ell''m''} - 2i(\delta_d\tilde{h}_{ab}^{\ell''m''} - \delta_{(a}\tilde{h}_{b)d}^{\ell''m''})]}{2r^2}, \tag{D4b}$$

$$\mathcal{B}_{a+}^{\ell'm'1\ell''m''0} = -\frac{(\sigma_+\tilde{h}_\circ^{\ell'm'}r_a + iM\sigma_-\tilde{h}_{a-}^{\ell'm'})\tilde{h}_\circ^{\ell''m''}}{r^5} + \frac{(\sigma_+\delta_a\tilde{h}_\circ^{\ell'm'} + i\sigma_-\lambda_{\ell',1}^2\tilde{h}_{a-}^{\ell'm'})\tilde{h}_\circ^{\ell''m''}}{2r^4}$$
$$+ \frac{\sigma_+[3\lambda_{\ell'',1}^2\tilde{h}_{b-}^{\ell'm'}(g^{bc}\tilde{h}_{c-}^{\ell''m''}r_a - r^b\tilde{h}_{a-}^{\ell''m''}) - r^b\tilde{h}_{ab}^{\ell'm'}\tilde{h}_\circ^{\ell''m''}]}{2r^3} + \sigma_+g^{bd}g^{ce}\tilde{h}_{bc}^{\ell''m''}\delta_{[a}\tilde{h}_{d]e}^{\ell'm'}$$
$$+ \frac{i\sigma_-[\tilde{h}_\circ^{\ell''m''}r^b\delta_{[a}\tilde{h}_{b]-}^{\ell'm'} - g^{bc}\tilde{h}_{b-}^{\ell'm'}(M\tilde{h}_{ac}^{\ell''m''} + r_{(a}\delta_{c)}\tilde{h}_\circ^{\ell''m''})]}{r^3} + i\sigma_-g^{cd}\delta^b\delta_{[a}\tilde{h}_{c]-}^{\ell'm'}\tilde{h}_{bd}^{\ell''m''}$$
$$+ \frac{6\sigma_+\lambda_{\ell'',1}^2g^{bc}\tilde{h}_{b-}^{\ell'm'}\delta_{[c}\tilde{h}_{a]-}^{\ell''m''} - i\sigma_-g^{bc}\tilde{h}_{b-}^{\ell'm'}(\lambda_{\ell'',1}^2\tilde{h}_{ac}^{\ell''m''} - 2\delta_c\delta_a\tilde{h}_\circ^{\ell''m''})}{4r^2} + \frac{\sigma_+g^{bd}g^{ce}r_{[b}\tilde{h}_{a]c}^{\ell'm'}\tilde{h}_{de}^{\ell''m''}}{r}$$
$$+ \frac{i\sigma_-g^{cd}[2(r^b\delta_{(a}\tilde{h}_{c)-}^{\ell'm'} - r_a\delta^b\tilde{h}_{c-}^{\ell'm'})\tilde{h}_{bd}^{\ell''m''} - \tilde{h}_{c-}^{\ell'm'}r^b(2\delta_{(a}\tilde{h}_{d)b}^{\ell''m''} - \delta_b\tilde{h}_{ad}^{\ell''m''})]}{2r}, \tag{D4c}$$

$$\mathcal{B}_{a+}^{\ell'm'2\ell''m''-1} = \frac{g^{bc}\tilde{h}_{b-}^{\ell''m''}(i\sigma_-\tilde{h}_{ac}^{\ell'm'} - 2\sigma_+\delta_{(a}\tilde{h}_{c)-}^{\ell'm'})}{4r^2}, \tag{D4d}$$

$$\mathcal{B}_\circ^{\ell'm'0\ell''m''0} = -\frac{1}{2}\lambda_{\ell',1}^2g^{ac}g^{bd}\tilde{h}_{ab}^{\ell'm'}\tilde{h}_{cd}^{\ell''m''} - \frac{\tilde{h}_\circ^{\ell'm'}\tilde{h}_\circ^{\ell''m''}(2f + \lambda_{\ell',1}^2)}{r^4} + \frac{2\tilde{h}_\circ^{\ell''m''}r^a\delta_a\tilde{h}_\circ^{\ell'm'}}{r^3} + \tilde{h}_{ab}^{\ell''m''}\delta^b\delta^a\tilde{h}_\circ^{\ell'm'}$$
$$- \frac{2Mg^{ac}g^{bd}\tilde{h}_{ab}^{\ell'm'}\tilde{h}_{cd}^{\ell''m''} + 2\tilde{h}_{ab}^{\ell''m''}r^a\delta^b\tilde{h}_\circ^{\ell'm'}}{r} + rr^ag^{bd}g^{ce}\tilde{h}_{bc}^{\ell''m''}(\delta_a\tilde{h}_{de}^{\ell'm'} - 2\delta_e\tilde{h}_{ad}^{\ell'm'}), \tag{D4e}$$

$$\mathcal{B}_\circ^{\ell'm'1\ell''m''-1} = \frac{2Mg^{ab}\tilde{h}_{a-}^{\ell'm'}\tilde{h}_{b-}^{\ell''m''} - ir^a(\tilde{h}_{a-}^{\ell''m''}\tilde{h}_\circ^{\ell'm'} - \tilde{h}_{a-}^{\ell'm'}\tilde{h}_\circ^{\ell''m''})}{r^3} - \frac{2r^ar^b\tilde{h}_{a-}^{\ell'm'}\tilde{h}_{b-}^{\ell''m''}}{r^2}$$
$$- \frac{2i(\tilde{h}_{a-}^{\ell'm'}\delta^a\tilde{h}_\circ^{\ell''m''} - \tilde{h}_{a-}^{\ell''m''}\delta^a\tilde{h}_\circ^{\ell'm'}) - (4f + \mu_{\ell'}^2 + \mu_{\ell''}^2 + \lambda_{\ell',1}^2 + \lambda_{\ell'',1}^2)g^{ab}\tilde{h}_{a-}^{\ell'm'}\tilde{h}_{b-}^{\ell''m''}}{4r^2}$$
$$+ \frac{g^{ab}r^c[\tilde{h}_{a-}^{\ell''m''}(2\delta_{[b}\tilde{h}_{c]-}^{\ell'm'} - i\tilde{h}_{bc}^{\ell'm'}) + \tilde{h}_{a-}^{\ell'm'}(2\delta_{[b}\tilde{h}_{c]-}^{\ell''m''} + i\tilde{h}_{bc}^{\ell''m''})]}{2r}, \tag{D4f}$$

$$\mathcal{B}_+^{\ell'm'1\ell''m''1} = -\frac{2i\sigma_-r^a\tilde{h}_{a-}^{\ell''m''}\tilde{h}_\circ^{\ell'm'}}{r^3} + \frac{\sigma_+[4r^ar^b - g^{ab}(2f + \mu_{\ell'}^2 + \lambda_{\ell',1}^2)]\tilde{h}_{a-}^{\ell'm'}\tilde{h}_{b-}^{\ell''m''} + 2i\sigma_-\tilde{h}_{a-}^{\ell''m''}\delta^a\tilde{h}_\circ^{\ell'm'}}{2r^2}$$
$$+ \frac{r^ag^{bc}\tilde{h}_{c-}^{\ell''m''}(2\sigma_+\delta_{[a}\tilde{h}_{b]-}^{\ell'm'} - i\sigma_-\tilde{h}_{ab}^{\ell'm'})}{r}, \tag{D4g}$$

$$\mathcal{B}_+^{\ell'm'2\ell''m''0} = \frac{1}{2}\tilde{h}_{ab}^{\ell''m''}g^{ac}(\sigma_+g^{bd}\tilde{h}_{cd}^{\ell'm'} + 2i\sigma_-\delta^b\tilde{h}_{c-}^{\ell'm'}). \tag{D4h}$$

The quantities appearing in Eq. (173) are

$$\mathcal{C}_{ab}^{\ell'm'0\ell''m''0} = 2\delta_{(a}\tilde{h}_{b)c}^{\ell'm'}\delta^c\tilde{h}_\bullet^{\ell''m''} - \delta_c\tilde{h}_{ab}^{\ell''m''}\delta^c\tilde{h}_\bullet^{\ell'm'} - \frac{\delta_c\tilde{h}_{ab}^{\ell''m''}\delta^c\tilde{h}_\circ^{\ell'm'} - 2\delta_{(a}\tilde{h}_{b)c}^{\ell'm'}\delta^c\tilde{h}_\circ^{\ell''m''}}{r^2} - \frac{2r^cg^{de}\tilde{h}_{cd}^{\ell''m''}(2\delta_{(a}\tilde{h}_{b)e}^{\ell'm'} - \delta_e\tilde{h}_{ab}^{\ell'm'})}{r}$$
$$- g^{cd}(2\delta_{(a}\tilde{h}_{b)c}^{\ell'm'} - \delta_c\tilde{h}_{ab}^{\ell'm'})\delta^e\tilde{h}_{de}^{\ell''m''}, \tag{D5a}$$

$$\mathcal{C}^{\ell'm'1\ell''m''-1}_{ab} = \frac{r^c[\tilde{h}^{\ell''m''}_{c-}(2\delta_{(a}\tilde{h}^{\ell'm'}_{b)-} + i\tilde{h}^{\ell'm'}_{ab}) + \tilde{h}^{\ell'm'}_{c-}(2\delta_{(a}\tilde{h}^{\ell''m''}_{b)-} - i\tilde{h}^{\ell''m''}_{ab})]}{r^3} + \frac{(\tilde{h}^{\ell''m''}_{ab} + 2i\delta_{(a}\tilde{h}^{\ell''m''}_{b)-})(\tilde{h}^{\ell'm'}_{\bullet} - i\delta^c\tilde{h}^{\ell'm'}_{c-}) + (\tilde{h}^{\ell'm'}_{ab} - 2i\delta_{(a}\tilde{h}^{\ell'm'}_{b)-})(\tilde{h}^{\ell''m''}_{\bullet} + i\delta^c\tilde{h}^{\ell''m''}_{c-})}{2r^2}, \tag{D5b}$$

$$\begin{aligned}\mathcal{C}^{\ell'm'1\ell''m''0}_{a+} = &-\frac{2i\sigma_- r_a r^b\tilde{h}^{\ell'm'}_{b-}\tilde{h}^{\ell''m''}_{\circ}}{r^4} + \frac{\sigma_+(\lambda^2_{\ell'',1}r^b\tilde{h}^{\ell'm'}_{b-}\tilde{h}^{\ell''m''}_{a-} - r_a\tilde{h}^{\ell'm'}_{\bullet}\tilde{h}^{\ell''m''}_{\circ})}{r^3} \\ &+ \frac{i\sigma_-[r^b\tilde{h}^{\ell'm'}_{b-}\delta_a\tilde{h}^{\ell''m''}_{\circ} - r_a(\tilde{h}^{\ell''m''}_{\circ}\delta^b\tilde{h}^{\ell'm'}_{b-} - \tilde{h}^{\ell'm'}_{b-}\delta^b\tilde{h}^{\ell''m''}_{\circ})]}{r^3} + \frac{1}{2}(\sigma_+\tilde{h}^{\ell'm'}_{ab} + i\sigma_-\delta_b\tilde{h}^{\ell'm'}_{a-})\delta^b\tilde{h}^{\ell''m''}_{\bullet} \\ &+ \frac{i\sigma_-[\delta_a\tilde{h}^{\ell''m''}_{\circ}\delta^b\tilde{h}^{\ell'm'}_{b-} + 2\delta^b\tilde{h}^{\ell''m''}_{\circ}\delta_{[b}\tilde{h}^{\ell'm'}_{a]-} - 4r_a r^b g^{cd}\tilde{h}^{\ell''m''}_{bc}\tilde{h}^{\ell'm'}_{d-} - \lambda^2_{\ell'',1}\tilde{h}^{\ell''m''}_{a-}\tilde{h}^{\ell'm'}_{\bullet}]}{2r^2} \\ &+ \frac{\sigma_+[\tilde{h}^{\ell'm'}_{\bullet}\delta_a\tilde{h}^{\ell''m''}_{\circ} + \lambda^2_{\ell'',1}\tilde{h}^{\ell''m''}_{a-}\delta^b\tilde{h}^{\ell'm'}_{b-} + \tilde{h}^{\ell'm'}_{ab}\delta^b\tilde{h}^{\ell''m''}_{\circ}]}{2r^2} - \frac{1}{2}\sigma_+ g^{bc}\tilde{h}^{\ell'm'}_{ab}\delta^d\tilde{h}^{\ell''m''}_{cd} - \frac{1}{2}i\sigma_-(\delta_a\tilde{h}^{\ell'm'}_{b-}\delta^b\tilde{h}^{\ell''m''}_{\bullet} \\ &+ 2g^{bc}\delta_{[b}\tilde{h}^{\ell'm'}_{a]-}\delta^d\tilde{h}^{\ell''m''}_{cd}) - \frac{\sigma_+ g^{bc}r^d\tilde{h}^{\ell'm'}_{ab}\tilde{h}^{\ell''m''}_{cd} - i\sigma_-[r_a\tilde{h}^{\ell'm'}_{b-}(\delta^b\tilde{h}^{\ell''m''}_{\bullet} - g^{bc}\delta^d\tilde{h}^{\ell''m''}_{cd}) + 2g^{bc}r^d\delta_{[a}\tilde{h}^{\ell'm'}_{b]-}\tilde{h}^{\ell''m''}_{cd}]}{r},\end{aligned} \tag{D5c}$$

$$\mathcal{C}^{\ell'm'0\ell''m''0}_{\circ} = \delta^a\tilde{h}^{\ell''m''}_{\circ}\delta^b\tilde{h}^{\ell'm'}_{ab} - 4r^a r^b g^{cd}\tilde{h}^{\ell'm'}_{ac}\tilde{h}^{\ell''m''}_{bd} - \delta_a\tilde{h}^{\ell'm'}_{\circ}\delta^a\tilde{h}^{\ell''m''}_{\bullet} + 2rr^a(\tilde{h}^{\ell''m''}_{ab}\delta^b\tilde{h}^{\ell'm'}_{\bullet} - g^{bc}\tilde{h}^{\ell''m''}_{ab}\delta^d\tilde{h}^{\ell'm'}_{cd}) - \frac{\delta_a\tilde{h}^{\ell''m''}_{\circ}\delta^a\tilde{h}^{\ell'm'}_{\circ}}{r^2} + \frac{4\tilde{h}^{\ell''m''}_{ab}r^a\delta^b\tilde{h}^{\ell'm'}_{\circ}}{r}, \tag{D5d}$$

$$\mathcal{C}^{\ell'm'1\ell''m''-1}_{\circ} = \frac{4r^a r^b\tilde{h}^{\ell'm'}_{a-}\tilde{h}^{\ell''m''}_{b-}}{r^2} + \frac{r^a[\tilde{h}^{\ell''m''}_{a-}(\delta^b\tilde{h}^{\ell'm'}_{b-} + i\tilde{h}^{\ell'm'}_{\bullet}) + \tilde{h}^{\ell'm'}_{a-}(\delta^b\tilde{h}^{\ell''m''}_{b-} - i\tilde{h}^{\ell''m''}_{\bullet})]}{r}, \tag{D5e}$$

$$\mathcal{C}^{\ell'm'1\ell''m''1}_{+} = \frac{2i\sigma_- r^a\tilde{h}^{\ell''m''}_{a-}\tilde{h}^{\ell'm'}_{\circ}}{r^3} + \frac{\tilde{h}^{\ell'm'}_{\circ}(\sigma_+\tilde{h}^{\ell''m''}_{\bullet} + i\sigma_-\delta^a\tilde{h}^{\ell''m''}_{a-})}{r^2}, \tag{D5f}$$

$$\mathcal{C}^{\ell'm'2\ell''m''0}_{+} = \frac{2i\sigma_- r^a g^{bc}\tilde{h}^{\ell''m''}_{ab}\tilde{h}^{\ell'm'}_{c-}}{r} - \frac{i\sigma_-\tilde{h}^{\ell'm'}_{a-}\delta^a\tilde{h}^{\ell''m''}_{\circ}}{r^2} - i\sigma_-\tilde{h}^{\ell'm'}_{a-}(\delta^a\tilde{h}^{\ell''m''}_{\bullet} - g^{ab}\delta^c\tilde{h}^{\ell''m''}_{bc}). \tag{D5g}$$

3. Stress-energy terms

The mode decomposition of Eq. (175) is

$$\tilde{\mathcal{T}}^{(2)\ell m}_{ab} = \tilde{T}^{(2)\ell m}_{ab} - g_{ab}(\tilde{T}^{(2)\ell m}_{\bullet} + r^{-2}\tilde{T}^{(2)\ell m}_{\circ}) + \sum_{\substack{\ell'm'\\ \ell''m''}}\sum_{s'=0,1}\lambda_{\ell',s'}\lambda_{\ell'',s'}C^{\ell m0}_{\ell'm's'\ell''m'',-s'}\mathcal{T}^{\ell'm's'\ell''m'',-s'}_{ab}, \tag{D6a}$$

$$\tilde{\mathcal{T}}^{(2)\ell m}_{a\pm} = \tilde{T}^{(2)\ell m}_{a\pm} + \sum_{\substack{\ell'm'\\ \ell''m''}}\frac{\lambda_{\ell',1}}{\lambda_{\ell,1}}C^{\ell m1}_{\ell'm'1\ell''m''0}\mathcal{T}^{\ell'm'1\ell''m''0}_{a\pm}, \tag{D6b}$$

$$\tilde{\mathcal{T}}^{(2)\ell m}_{\circ} = -r^2\tilde{T}^{(2)\ell m}_{\bullet} + \sum_{\substack{\ell'm'\\ \ell''m''}}\sum_{s'=0,1}\lambda_{\ell',s'}\lambda_{\ell'',s'}C^{\ell m0}_{\ell'm's'\ell''m'',-s'}\mathcal{T}^{\ell'm's'\ell''m'',-s'}_{\circ}, \tag{D6c}$$

$$\tilde{\mathcal{T}}^{(2)\ell m}_{\pm} = \tilde{T}^{(2)\ell m}_{\pm}. \tag{D6d}$$

The coupling functions $\mathcal{T}^{\ell'm's'\ell''m'',s''}_{\cdot}$ are

$$\mathcal{T}^{\ell'm'0\ell''m''0}_{ab} = \frac{1}{2}g_{ab}g^{ce}g^{df}\tilde{h}^{\ell'm'}_{cd}T^{\ell''m''}_{ef} - \frac{1}{2}\tilde{h}^{\ell'm'}_{ab}g^{cd}T^{\ell''m''}_{cd} + r^{-4}g_{ab}\tilde{h}^{\ell''m''}_{\circ}T^{\ell'm'}_{\circ} - r^{-2}\tilde{h}^{\ell''m''}_{ab}T^{\ell'm'}_{\circ}, \tag{D7a}$$

$$\mathcal{T}^{\ell'm'1\ell''m'',-1}_{ab} = -\frac{1}{2r^2}g_{ab}g^{cd}[\tilde{h}^{\ell''m''}_{c-}(T^{\ell'm'}_{d-} - iT^{\ell'm'}_{d+}) + \tilde{h}^{\ell'm'}_{c-}(T^{\ell''m''}_{d-} + iT^{\ell''m''}_{d+})], \tag{D7b}$$

$$\mathcal{T}^{\ell'm'1\ell''m''0}_{a+} = \frac{i}{4}\sigma_-\tilde{h}^{\ell'm'}_{a-}g^{bc}T^{\ell''m''}_{bc} + \frac{i}{2r^2}\sigma_-\tilde{h}^{\ell'm'}_{a-}T^{\ell''m''}_{\circ}, \tag{D7c}$$

$$\mathcal{T}^{\ell'm'0\ell''m''0}_{\circ} = \frac{1}{2}r^2g^{ac}g^{bd}\tilde{h}^{\ell'm'}_{ab}T^{\ell''m''}_{cd} - \frac{1}{2}\tilde{h}^{\ell'm'}_{\circ}g^{ab}T^{\ell''m''}_{ab} + r^{-2}\tilde{h}^{\ell''m''}_{\circ}T^{\ell'm'}_{\circ} - r^{-2}\tilde{h}^{\ell'm'}_{\circ}T^{\ell''m''}_{\circ}, \tag{D7d}$$

$$\mathcal{T}^{\ell'm'1\ell''m'',-1}_{\circ} = -\frac{1}{2}g^{ab}\left[\tilde{h}^{\ell''m''}_{a-}(T^{\ell'm'}_{b-} - iT^{\ell'm'}_{b+}) + \tilde{h}^{\ell'm'}_{a-}(T^{\ell''m''}_{b-} + iT^{\ell''m''}_{b+})\right]. \tag{D7e}$$

APPENDIX E: FIELD EQUATIONS FOR LOW MULTIPOLES

In this appendix we summarize the special cases of the field equations (176) for $\ell = 0$ and $\ell = 1$. We specifically discuss the $\ell = 0$ and odd-parity $\ell = 1$ equations, which we are able to relate to the evolution of mass and spin. We have not found a new or illuminating form for the even-parity $\ell = 1$ equations, which are associated with a displacement of the center of mass [55].

1. $\ell = 0$

The $\ell = 0$ field equations, with ℓm labels omitted for visual simplicity, are

$$\delta R_{ab}[\tilde{h}^{(1)}_{\cdot\cdot}] = 8\pi\mathcal{T}^{(1)}_{ab}, \tag{E1a}$$

$$\delta R_{\circ}[\tilde{h}^{(1)}_{\cdot\cdot}] = 8\pi\mathcal{T}^{(1)}_{\circ}, \tag{E1b}$$

and their analogs at second order. These can be written entirely in terms of the invariant variables $\tilde{h}_{rr}$ and φ defined in Eqs. (143) and (148). However, we opt to replace $\tilde{h}_{rr}$ with an effective mass perturbation δM, defined from

$$\tilde{h}_{rr} = \frac{\partial g_{rr}}{\partial M}\delta M = \frac{2\delta M}{rf^2}. \tag{E2}$$

In terms of δM and φ,

$$\delta R_{tt} = \frac{M\delta M}{fr^4} - \frac{\partial_t^2\delta M}{fr} - \frac{M\partial_r\delta M}{r^3} - \frac{f(2r-M)\varphi}{2r^2} - \frac{1}{2}f^2\partial_r\varphi, \tag{E3a}$$

$$\delta R_{tr} = \frac{2}{r^2 f}\frac{\partial\delta M}{\partial t}, \tag{E3b}$$

$$\delta R_{rr} = -\frac{2r-3M}{f^3r^4}\delta M + \frac{\partial_t^2\delta M}{f^3 r} + \frac{2r-3M}{f^2r^3}\partial_r\delta M + \frac{3M\varphi}{2f^2r^2} + \frac{1}{2}\partial_r\varphi, \tag{E3c}$$

$$\delta R_{\circ} = r^{-1}\partial_r(r\delta M) + \frac{2M}{r^2 f}\delta M + \frac{1}{2}rf\varphi. \tag{E3d}$$

We can further reduce these field equations by eliminating φ. Solving $\delta R_{\circ} = 8\pi\mathcal{T}_{\circ}$ for φ yields

$$\varphi = -\frac{2\partial_r\delta M}{rf} - \frac{2\delta M}{r^2f^2} + \frac{16\pi\mathcal{T}_{\circ}}{rf}, \tag{E4}$$

which reduces the remaining three components of the field equations to equations for δM. The tr component, $\delta R_{tr} = 8\pi\mathcal{T}_{tr}$, reads

$$\frac{\partial}{\partial t}\delta M = 4\pi r^2 f T_{tr}, \tag{E5}$$

where we have used $\mathcal{T}_{tr} = T_{tr}$. Equation (E5) is a flux-balance equation, equating the rate of change of the mass at radius r to the flux of energy crossing the $r = \text{const}$ surface. This determines δM up to a time-independent function of r. The function of r can be determined up to a constant from the "antitrace" piece of the field equations,

$$f^{-1}\delta R_{tt} + f\delta R_{rr} = 8\pi(f^{-1}\mathcal{T}_{tt} + f\mathcal{T}_{rr}), \tag{E6}$$

which can be simplified to

$$\frac{\partial}{\partial r}\delta M = 4\pi r^2 f^{-1}T_{tt} \tag{E7}$$

after using (E4) and expressing $\mathcal{T}_{\alpha\beta}$ in terms of $T_{\alpha\beta}$. Equation (E7) relates the mass within a sphere of radius r to the total energy within that sphere. Equations (E5) and (E7) together determine δM up to a constant δM_0, corresponding to a trivial perturbation toward another Schwarzschild solution with mass $M + \epsilon\delta M_0$.

In this way, the entire invariant content of the $\ell = 0$ solution is placed in δM, which satisfies physical energy-balance equations. The remaining piece of the field equations is the trace piece,

$$\frac{1}{2}g^{ab}\delta R_{ab} = 4\pi g^{ab}\mathcal{T}_{ab} \coloneqq 8\pi\mathcal{T}_{\bullet}. \tag{E8}$$

After using Eq. (E4), we can simplify this to a wave equation for δM,

$$\Box_{\mathcal{M}^2}\delta M = 8\pi\left(f\partial_r\mathcal{T}_\circ + \frac{M}{r^2}\mathcal{T}_\circ - rf\mathcal{T}_\bullet\right). \tag{E9}$$

This final equation is redundant due to the Bianchi identities, but it shows that the mass perturbation propagates causally according to a hyperbolic equation.

The same calculations apply at second order with the obvious replacements of source terms. As a final comment in this section, we note that at second order the quadratic source terms dramatically simplify for $\ell = 0$ due to Eq. (96). Equation (171), for example, reduces to

$$\sum_{s'=0}^{s'_{\max}}\sum_{\ell'=s'}^{\infty}\sum_{m'=-\ell'}^{+\ell'}\lambda_{\ell',s'}\lambda_{\ell'',s'}\frac{(-1)^{m'+s'}}{\sqrt{4\pi}}\mathcal{A}^{\ell'm's'\ell',-m',-s'}_{\cdot}. \tag{E10}$$

2. $\ell = 1$, odd parity

The $\ell = 1$, odd-parity field equations, with ℓm labels omitted for visual simplicity, are

$$\delta R_{a-}[\tilde{h}^{(1)}_{\cdot}] = 8\pi\mathcal{T}^{(1)}_{a-}, \tag{E11}$$

and their analogs at second order. These can be written entirely in terms of the invariant variable φ_- defined in Eq. (165). However, we opt to write it in terms of an effective angular momentum variable δJ defined by

$$\varphi_- = \frac{\delta J}{r^4}. \tag{E12}$$

Explicitly, the field equations reduce to

$$\frac{\partial}{\partial r}\delta J = -\frac{16\pi r^2}{f}T_{t-}, \tag{E13a}$$

$$\frac{\partial}{\partial t}\delta J = -16\pi r^2 f T_{r-}. \tag{E13b}$$

In analogy with Eqs. (E5) and (E7), Eq. (E13b) can be interpreted as the statement that the angular momentum within a sphere of radius r changes at a rate equal to the instantaneous flux of angular momentum into the sphere, while Eq. (E13a) can be interpreted as the statement that the total angular momentum within the sphere is equal to the integrated angular momentum density within the sphere. These two equations determine δJ up to a constant. The constant represents a perturbation toward a Kerr solution with spin parameter $\frac{\delta J}{M}$.

In analogy with Eq. (E9), from Eq. (E13) we can derive a wave equation for δJ:

$$\Box_{\mathcal{M}^2}\delta J = -16\pi\epsilon^{ab}\delta_a(r^2 T_{b-}). \tag{E14}$$

APPENDIX F: FIELD EQUATIONS IN BARACK-LOUSTO-SAGO CONVENTIONS

For self-force computations in the Lorenz gauge, the most common set of conventions are those of Barack and Lousto [69] as modified by Barack and Sago [70].[4] These conventions were used at first order in Refs. [70,110,111] (among others) and in all second-order calculations [30,56,57,109]. In this appendix we describe the translation of our results into these conventions.

The Barack-Lousto-Sago conventions use a set of harmonics $Y^{i\ell m}_{\mu\nu}$, where i runs from 1 to 10, with nonvanishing components given by

$$Y^{1\ell m}_{ab} = \frac{1}{\sqrt{2}}(t_a t_b + f^{-2} r_a r_b)Y^{\ell m}, \tag{F1a}$$

$$Y^{2\ell m}_{ab} = \frac{f^{-1}}{\sqrt{2}}(t_a r_b + r_a t_b)Y^{\ell m}, \tag{F1b}$$

$$Y^{3\ell m}_{ab} = -\frac{1}{\sqrt{2}}g_{ab}Y^{\ell m}, \tag{F1c}$$

$$Y^{4\ell m}_{aA} = \frac{r}{\sqrt{2}\lambda_{\ell,1}}t_a Y^{\ell m}_A, \tag{F1d}$$

$$Y^{5\ell m}_{aA} = \frac{rf^{-1}}{\sqrt{2}\lambda_{\ell,1}}r_a Y^{\ell m}_A, \tag{F1e}$$

$$Y^{6\ell m}_{AB} = \frac{r^2}{\sqrt{2}}\Omega_{AB}Y^{\ell m}, \tag{F1f}$$

$$Y^{7\ell m}_{AB} = \frac{\sqrt{2}r^2}{\lambda_{\ell,2}}Y^{\ell m}_{AB}, \tag{F1g}$$

$$Y^{8\ell m}_{aA} = -\frac{r}{\sqrt{2}\lambda_{\ell,1}}t_a X^{\ell m}_A, \tag{F1h}$$

$$Y^{9\ell m}_{aA} = -\frac{rf^{-1}}{\sqrt{2}\lambda_{\ell,1}}r_a X^{\ell m}_A, \tag{F1i}$$

$$Y^{10\ell m}_{AB} = -\frac{\sqrt{2}r^2}{\lambda_{\ell,2}}X^{\ell m}_{AB}. \tag{F1j}$$

These harmonics are orthogonal (but not orthonormal) with respect to the inner product $\langle S_{\mu\nu}, Q_{\mu\nu}\rangle \coloneqq \int \eta^{\alpha\mu}\eta^{\beta\nu}S^*_{\alpha\beta}Q_{\mu\nu}d\Omega$, where $\eta^{\mu\nu} \coloneqq \mathrm{diag}(1, f^2, r^{-2}\Omega^{AB})$.[5] If we expand a tensor $v_{\mu\nu}$ as

[4]The Barack-Lousto-Sago basis is related to the Barack-Lousto basis by $Y^{3\ell m(BLS)}_{\mu\nu} = fY^{3\ell m(BL)}_{\mu\nu}$, leading to coefficients related by $S^{(BL)}_{3\ell m} = fS^{(BLS)}_{3\ell m}$.

[5]The definition of $\eta^{\mu\nu}$ corrects a typo in Ref. [69], as previously noted in Ref. [110].

$$v_{\mu\nu} = \sum_{i\ell m} v_{i\ell m} Y^{i\ell m}_{\mu\nu}, \tag{F2}$$

then the coefficients are given by[6]

$$v_{i\ell m} = \kappa_i \int Y^{i\ell m*}_{\alpha\beta} \eta^{\alpha\mu}\eta^{\beta\nu} v_{\mu\nu} d\Omega, \tag{F3}$$

where $\kappa_3 = f^{-2}$ and $\kappa_i = 1$ for $i \neq 3$.

An advantage of these harmonics is that they are well suited to assessing (or imposing) the regularity of a tensor at the future horizon. A tensor $v_{\mu\nu} = \sum_{i\ell m} v_{i\ell m} Y^{i\ell m}_{\mu\nu}$ has continuous components in ingoing Eddington-Finkelstein coordinates (v, r) at $r = 2M$ if and only if

(1) each coefficient $v_{i\ell m}$ is continuous there,
(2) $v_{2\ell m} = v_{1\ell m} + \mathcal{O}(f^2)$, and
(3) $v_{i\ell m} = v_{i+1,\ell m} + \mathcal{O}(f)$ for $i = 4, 8$.

If each $v_{i\ell m}$ is a smooth function of v and r at $r = 2M$, then the above conditions are equivalent to smoothness of $v_{\mu\nu}$ at the future horizon.

Another advantage of this set of harmonics is that it makes trace reversals trivial. If we expand a tensor $v_{\mu\nu}$ as in Eq. (F2) and its trace reverse as $\bar{v}_{\mu\nu} = \sum_{i\ell m} \bar{v}_{i\ell m} Y^{i\ell m}_{\mu\nu}$, then the coefficients in the two expansions are related by

$$\bar{v}_{i\ell m} = v_{i\ell m} \quad \text{if } i \neq 3, 6, \tag{F4a}$$

$$\bar{v}_{3\ell m} = v_{6\ell m}, \tag{F4b}$$

$$\bar{v}_{6\ell m} = v_{3\ell m}. \tag{F4c}$$

Hence, a trace reversal is accomplished by the simple switch $i = 3 \leftrightarrow i = 6$.

The coefficients $v_{i\ell m}$ are related to the tensor-harmonic coefficients in the body of the paper according to

$$v_{1\ell m} = \frac{1}{\sqrt{2}}(v^{\ell m}_{tt} + f^2 v^{\ell m}_{rr}), \tag{F5a}$$

$$v_{2\ell m} = \sqrt{2} f v^{\ell m}_{tr}, \tag{F5b}$$

$$v_{3\ell m} = -\frac{1}{\sqrt{2}} g^{ab} v^{\ell m}_{ab}, \tag{F5c}$$

$$v_{4\ell m} = \frac{\sqrt{2}\lambda_{\ell,1}}{r} v^{\ell m}_{t+}, \tag{F5d}$$

$$v_{5\ell m} = \frac{\sqrt{2}\lambda_{\ell,1} f}{r} v^{\ell m}_{r+}, \tag{F5e}$$

$$v_{6\ell m} = \frac{\sqrt{2}}{r^2} v^{\ell m}_{\circ}, \tag{F5f}$$

$$v_{7\ell m} = \frac{\lambda_{\ell,2}}{\sqrt{2} r^2} v^{\ell m}_{+}, \tag{F5g}$$

$$v_{8\ell m} = -\frac{\sqrt{2}\lambda_{\ell,1}}{r} v^{\ell m}_{t-}, \tag{F5h}$$

$$v_{9\ell m} = -\frac{\sqrt{2}\lambda_{\ell,1} f}{r} v^{\ell m}_{r-}, \tag{F5i}$$

$$v_{10\ell m} = -\frac{\lambda_{\ell,2}}{\sqrt{2} r^2} v^{\ell m}_{-}. \tag{F5j}$$

These relations can be used to obtain the linear and quadratic quantities in the Lorenz-gauge field equations ($\mathcal{E}_{i\ell m}$, $\mathcal{A}_{i\ell m}$, and $\mathcal{B}_{i\ell m}$) from their counterparts $\mathcal{E}^{\ell m}_{\cdot}$, $\mathcal{A}^{\ell m}_{\cdot}$, and $\mathcal{B}^{\ell m}_{\cdot}$ given in the body of the paper. However, the results will be expressed in terms of the field variables $h^{\ell m}_{\cdot}$, which must be translated to Barack-Lousto-Sago variables.

Instead of directly using coefficients in an expansion of $h^{(n)}_{\mu\nu}$ of the form (F2), the Barack-Lousto-Sago convention is to scale those coefficients by convenient factors. Specifically, the trace-reversed field is expanded as

$$\bar{h}^{(n)}_{\mu\nu} = \frac{1}{r}\sum_{i\ell m} a_{i\ell} \bar{h}^{(n)}_{i\ell m} Y^{i\ell m}_{\mu\nu}, \tag{F6}$$

where

$$a_{i\ell} := \frac{1}{\sqrt{2}}\begin{cases} 1 & \text{for } i = 1, 2, 3, 6, \\ \frac{1}{\lambda_{\ell,1}} & \text{for } i = 4, 5, 8, 9, \\ \frac{1}{\lambda_{\ell,2}} & \text{for } i = 7, 10. \end{cases} \tag{F7}$$

The nth-order field variables are then the coefficients $\bar{h}^{(n)}_{i\ell m}$. We can express our field variables $h^{(n)\ell m}_{\cdot}$ in terms of these by inverting the relations (F5), accounting for the rescaling, and performing the trace reversal $i = 3 \leftrightarrow i = 6$. The result is given in Table II.

If we begin from a field equation of the form (27) and specialize to the Lorenz gauge, we reduce the equation to Eq. (28), reproduced here for convenience: $\mathcal{E}_{\mu\nu}[\bar{h}^{(n)}] = -2S^{(n)}_{\mu\nu}$. Obtaining $\mathcal{E}_{i\ell m}$ from $\mathcal{E}^{\ell m}_{\cdot}$ using Eq. (F5), substituting Eq. (F6) into $\mathcal{E}_{i\ell m}$, and then adding terms proportional to the gauge condition, as described in Ref. [69], leads to the Barack-Lousto-Sago formulation of the linearized Einstein equation in the Lorenz gauge, which is written as

$$\Box^{2d}_{\rm sc} \bar{h}^{(n)}_{i\ell m} + \mathcal{M}^{j}_{i\ell} \bar{h}^{(n)}_{j\ell m} = \frac{rf}{2a_{i\ell}} S^{(n)}_{i\ell m}. \tag{F8}$$

Here $\Box^{2d}_{\rm sc} = \partial_u\partial_v + V_\ell$ is a two-dimensional scalar wave operator with potential $V_\ell = \frac{1}{4} f[2M/r^3 + \ell(\ell+1)/r^2]$,

[6] This corrects Eq. (2.7) in Ref. [110], which omitted the factor of N_i, as previously noted in Ref. [109].

and the terms $\mathcal{M}^j_{i\ell}\bar{h}^{(1)}_{j\ell m}$ are given in Eqs. (A1)–(A10) of Ref. [70]. $S^{(n)}_{i\ell m}$ is obtained from $S^{(n)\ell m}_{\cdot}$ via Eq. (F5).

At first order, Eq. (F8) becomes

$$\Box^{2d}_{\rm sc}\bar{h}^{(1)}_{i\ell m} + \mathcal{M}^j_{i\ell}\bar{h}^{(1)}_{j\ell m} = \frac{4\pi r f}{a_{i\ell}} T^{(1)}_{i\ell m}. \tag{F9}$$

At second order, it becomes

$$\Box^{2d}_{\rm sc}\bar{h}^{(2)}_{i\ell m} + \mathcal{M}^j_{i\ell}\bar{h}^{(2)}_{j\ell m} = \frac{4\pi r f}{a_{i\ell}} T^{(2)}_{i\ell m} - \frac{rf}{2a_{i\ell}}\delta^2 G_{i\ell m}[h^{(1)}] \tag{F10}$$

or, more explicitly, in terms of the sources appearing in Sec. VI D,

$$\Box^{2d}_{\rm sc}\bar{h}^{(2)}_{i\ell m} + \mathcal{M}^j_{i\ell}\bar{h}^{(2)}_{j\ell m} = \frac{4\pi r f}{a_{i\ell}} \bar{\mathcal{T}}^{(2)}_{i\ell m} - \frac{rf}{4a_{i\ell}}(\bar{\mathcal{A}}_{i\ell m} + \bar{\mathcal{B}}_{i\ell m}). \tag{F11}$$

The source terms $\bar{\mathcal{T}}^{(2)}_{i\ell m}$, $\bar{\mathcal{A}}_{i\ell m}$, and $\bar{\mathcal{B}}_{i\ell m}$ can be obtained explicitly by (i) constructing $\mathcal{T}^{(2)}_{i\ell m}$, $\mathcal{A}_{i\ell m}$, and $\mathcal{B}_{i\ell m}$ from $\mathcal{T}^{(2)\ell m}_{\cdot}$, $\mathcal{A}^{\ell m}_{\cdot}$, and $\mathcal{B}^{\ell m}_{\cdot}$ using Eq. (F5), (ii) replacing the variables $h^{(1)\ell m}_{\cdot}$ with the variables $\bar{h}^{(1)}_{i\ell m}$ using Table II, and (iii) performing the trace reversal $i = 3 \leftrightarrow i = 6$ of $\mathcal{T}^{(2)}_{i\ell m}$, $\mathcal{A}_{i\ell m}$, and $\mathcal{B}_{i\ell m}$ to obtain $\bar{\mathcal{T}}^{(2)}_{i\ell m}$, $\bar{\mathcal{A}}_{i\ell m}$, and $\bar{\mathcal{B}}_{i\ell m}$.

In self-force computations, $T^{(1)}_{\mu\nu}$ is the stress-energy tensor of a point mass. At second order, rather than working with a stress-energy tensor and solving directly for the physical retarded field, we instead use a puncture scheme. A singular piece of the metric perturbation, representing the particle's local self-field that diverges at the particle's position, is moved to the right-hand side of the field equation, and one solves for the regular residual field. The field equations in that case then become

$$\Box^{2d}_{sc}\bar{h}^{(2)\mathcal{R}}_{i\ell m} + \mathcal{M}^j_{i\ell}\bar{h}^{(2)\mathcal{R}}_{j\ell m} = -(\Box^{2d}_{sc}\bar{h}^{(2)\mathcal{P}}_{i\ell m} + \mathcal{M}^j_{i\ell}\bar{h}^{(2)\mathcal{P}}_{j\ell m}) - \frac{rf}{4a_{i\ell}}(\bar{\mathcal{A}}_{i\ell m} + \bar{\mathcal{B}}_{i\ell m}), \tag{F12}$$

where $\bar{h}^{(2)\mathcal{P}}_{i\ell m}$ are the harmonic coefficients in the expansion of the 4D puncture field given in Ref. [53], and $\bar{h}^{(2)\mathcal{R}}_{i\ell m} \coloneqq \bar{h}^{(2)}_{i\ell m} - \bar{h}^{(2)\mathcal{P}}_{i\ell m}$ are the residual field modes. No stress-energy terms appear in Eq. (F12), and the total source on the right-hand side is defined on the puncture's worldline by taking the limit from off the worldline; see the discussion around Eqs. (13)–(17) in Ref. [112]. The field equations are also further modified using a two-timescale expansion, as described in Ref. [109].

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