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The Second Order Close Limit Approximation

Towards exploring nonlinear behaviour at the horizon

Thesis MSc Physics and Astronomy

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Abstract:
The nonlinear nature of general relativity complicates the development of analytical models for the merging phase of black hole binaries, necessitating reliance on numerical simulations and obscuring the underlying physics. Recent studies on the ringdown phase have highlighted the need to incorporate second-order, nonlinear modes. In response, we utilize second-order black hole perturbation theory within the close limit approximation to model nonlinearities during the merger phase, which determine the "initial data" for the subsequent ringdown phase. Our primary aim is to connect horizon physics with gravitational wave signals. This thesis provides a detailed guide for analytically setting up the second-order close limit approximation. Focusing on a black hole binary in a head-on collision, we derive a second-order Zerilli equation where first-order perturbations act quadratically as a source term. We discuss deviations from existing literature and suggest potential extensions to the framework.

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1 Introduction

The direct detection of gravitational waves (GWs) by the LIGO-VIRGO-Kagra collaboration has opened up a new frontier for exploring gravity [1]. While these detections of coalescing black holes have provided invaluable insights, they have also posed new questions. One of them being the unexpectedly well-behaved GW signal during the violent merger phase. By nature, general relativity (GR) is a nonlinear theory with all kinds of self-interactions and unpredictable behaviour. This non-linearity complicates the prediction of events due to the difficulty in finding exact solutions. During the merger phase, characterized by highly deformed spacetimes, these nonlinearities are expected to be crucial. However, so far linear approximations have been in surprising agreement with observations and simulations. This begs the question where the nonlinearities are hiding.

Recent inquiries into numerical simulations of black hole (BH) collisions have indicated the presence of nonlinear modes in the final stages of the coalescence of a binary black hole (BBH), known as the ringdown phase [2, 3]. This signifies that the nonlinear dynamics of the system cannot simply be ignored. Since we do not have exact physical solutions for two BHs, we have to rely on approximations to make analytical predictions. In the ringdown phase, the system's spacetime is treated as a perturbation of the final BH's spacetime. Currently, BH perturbation theory in this stage is only carried out up to first order [4], thereby neglecting all nonlinear interactions. The recent developments regarding the ringdown phase establish that these nonlinear interactions are essential and that the perturbation theory should be extended to include second order contributions.

Our goal is to better understand the role of nonlinearities during the preceding merger phase and determine whether they reveal new physics. Specifically, we aim to investigate if processes near the horizon can be related to the GW waveform observed at infinity. This would allow us to use GW signals as a direct probe for the nonlinear nature of GR and provide a better grasp of the physics involved in BBH merger. Motivated by the recent developments for the successive ringdown phase, we also adopt a second order perturbative framework for the merger phase, utilising the close limit approximation (CLA) [5] to incorporate the first set of nonlinear self-interactions and analyse their behaviour.

1.1 Nonlinearities in GWs

A typical time-domain waveform from the coalescence of two BHs can be divided into three stages: the inspiral, the merger and the ringdown. Roughly speaking, the inspiral features a regular sinusoid with an increasing frequency that is generated as the BHs orbit each other at large separations, gradually edging closer towards each other as they slowly emit some of their energy in the form of GWs. When the binary system closes in on itself, the amplitude of the GW signal rises steeply as the two BHs fuse into a single BH. This marks the merger phase. In the final phase, called the ringdown, the resultant single BH settles down into a Kerr BH by radiating its final deformations in the form of GWs.

The inspiral and ringdown phase are both quite well understood as approximate solutions in terms of perturbation theory. During the insprial when the BBH has a large separation, the system can be treated as flat spacetime with correction terms, modeled using post-Newtonian/post-Minkowskian (PN/PM) expansions, which have been developed to high orders [6, 7]. After the merger, the system can be described as a perturbation of a single BH spacetime such as Schwarzschild or Kerr. The GW signal in the ringdown phase is modelled as a superposition of damped oscillations, known as Quasinormal modes (QNMs) [4, 8]. However, the intermediate merger phase is notoriously challenging to describe analytically due to the strong fields, requiring extensive numerical relativity (NR) simulations that solve the fully nonlinear Einstein equations [9, 10]. This leaves us without a solid analytical foundation for this phase.

Furthermore, distinguishing the boundaries between these phases is difficult [11, 12]. Both the PN/PM expansion and QNMs have successfully predicted a GW signal that aligns with NR predictions, even when extended well into what could be considered to be the merger regime [13, 14]. This motivates the choice of using these approximations as a tool to analytically describe the merger phase. Since we are ultimately interested in horizon physics, we focus on using BH perturbation methods for the merger, which are more suitable for our purposes.

The description of the ringdown phase using BH perturbation theory is typically conducted only at first, linear order [4]. It has been suggested that this first order approximation is sufficient for describing the ringdown phase if enough overtones are included. However, recent studies have challenged this claim, suggesting this may be an artifact of overfitting, with the fit's accuracy varying depending on the starting times used. Studies like [2, 3] indicate that incorporating quadratic modes results in more robust fits that remain stable across different starting times, making a second-order framework necessary. Consequently, there has been a push to include second order effects.

In the ringdown phase, the wavefunction is treated as a superposition different QNMs. At first order, each QNM is characterised by a mode (ℓ, m, n), where ℓ and m denote the corresponding spherical harmonic and n the overtone number. The QNMs' frequencies $\omega_{\ell mn}$ depend on the final BH's mass and spin. The amplitudes $A_{\ell mn}$, on the other hand, depend on the parameters of the progenitor binary. Quadratic modes now arise from first order linear modes (ℓ_i, m_i, n_i) interacting with each other at second order, represented as $(\ell_1, m_1, n_1) \times (\ell_2, m_2, n_2)$. Their corresponding frequency is the sum or difference of the two linear QNM frequencies, and their amplitude is the product of the linear amplitudes and some complicated coupling coefficient. These quadratic QNMs could potentially be measured by future space-based GW detectors like LISA [15], providing a direct measurement of GR's nonlinear behaviour.

Taking inspiration from the developments regarding the ringdown phase, we adopt second order BH perturbation theory to model the merger phase. This framework allows us to explore horizon dynamics and incorporate some of GR's inherent nonlinearities. We consider systems described by a metric

$$g_{\mu\nu} = {}^{(0)}g_{\mu\nu} + \epsilon\, {}^{(1)}g_{\mu\nu} + \epsilon^2\, {}^{(2)}g_{\mu\nu} + \mathcal{O}(\epsilon^3), \tag{1.1}$$

where ${}^{(0)}g_{\mu\nu}$ is a background spacetime which is a solution to the vacuum Einstein equations and ϵ is some expansion parameter. We will always use the superscript (i) on the left of a quantity to indicate its perturbative order.

1.2 Close Limit Approximation

We specifically use the Close Limit Approximation (CLA), first proposed in [5], to model the merger phase. In this approach, the merging BBH is modelled by applying perturbation theory in the limit of small initial separation. In this limit, an apparent horizon encompasses both BHs, allowing us to treat the system as a deformation of a single BH spacetime, such as Schwarzschild or Kerr (see Fig. 1). This approximation has shown surprising agreement with numerical simulations, even when the expansion parameter is marginally small [16, 17].

The CLA was introduced in the 1990s as an alternative to the computationally expensive NR simulations,

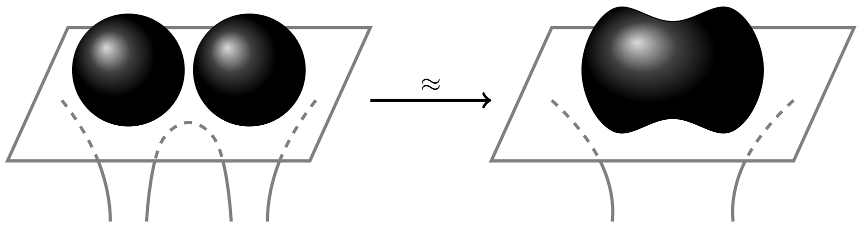


Figure 1: In the CLA, we treat a system of two BHs with a small initial separation as a perturbation of a single BH spacetime.

not readily available at the time. Most work has focused on collisions of non-rotating or slowly rotating BHs that settle into a single non-rotating BH, using Schwarzschild perturbation theory. Early calculations were conducted only up to first order [5, 18–21]. Later, the CLA was extended to second order [14, 22–26]. For a review of second-order treatment, see [16]. The extension to second order was primarily motivated as a tool to verify the accuracy of first-order predictions and determine the parameters for which the approximation was valid, essential at the time due to the limited availability of NR simulations for comparison.

With the advancement in computing and consequently NR, the need for accurate analytic models decreased, resulting in limited publications on the second order CLA since the early 2000s, apart from sporadic works [27–30]. The renewed interest in second order BH perturbation theory highlights a gap in research, with some original complex calculations no longer readily available. Therefore, this thesis aims to bridge this gap by providing a comprehensive overview of the analytical steps involved in setting up the second order CLA.

This thesis is organised as follows. We start by elaborating on the steps involved in the CLA and cover some theory necessary for carrying out the approximation in Sec. 2. In Sec. 3, we continue with an easy example of two initially static BHs up to first order to get a feeling for how the CLA is set up. Then, we present the main calculations done in this project in Sec. 4, where we discuss two BHs in a the head-on collision. We conclude in Sec. 5 with a consise summary and an outlook of further steps that have to be undertaken to get to an analytical description of the merger phase and we make recommendations for further research. This work is supplemented by extensive appendices App. A–C that elaborate on gauge transformations, the Einstein equations and the Regge-Wheeler-Zerilli formalism, all in the context of second order perturbation theory.

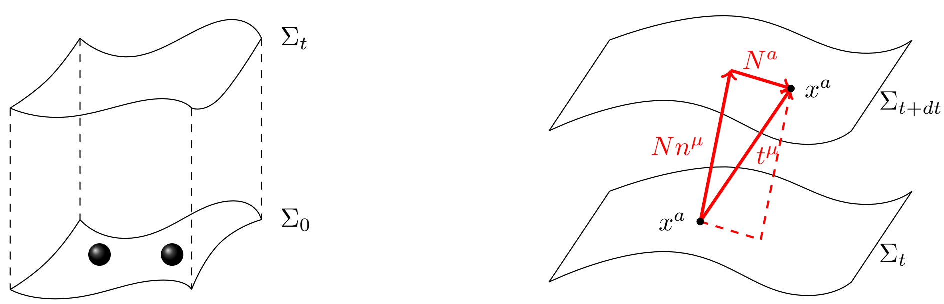
2 Close Limit Approximation

The CLA applies similar methods to NR to describe the evolution of a BBH and consequently its generated GW signal. Both use the ADM formalism (see [31]), also known as a 3+1 split, where a spacetime is sliced in a family of 3D surfaces, each representing a specific time instance. The CLA starts by specifying initial data on a 3D slice to represent the system at $t = 0$ and then evolving this initial data over time to obtain the full spacetime. However, while NR evolves the initial data using the fully nonlinear vacuum Einstein equations, the CLA evolves perturbations using master equations derived from the expanded Einstein equations. Setting up the CLA involves four primary steps (see Fig. 3): first, specifying initial data to represent the system. Second, extracting perturbations relative to a single black hole background by expanding in a small parameter related to the initial separation. Third, fixing these perturbations in a convenient gauge and finally, numerically integrating the master equation to determine the time evolution of the perturbations.

Throughout this work, we adopt a $(-+++)$ signature for the metric and use natural units, setting $c = G = 1$. Greek letters $\mu, \nu, \ldots$ indicate spacetime indices ranging over $0, 1, 2, 3$, while Latin letters $a, b, \ldots$ denote spatial indices ranging over $1, 2, 3$.

2.1 Initial Data

The first step in setting up the CLA is constructing suitable initial data to represent the BBH. This requires specifying a spatial 3-metric γ_{ab} and extrinsic curvature K_{ab} on some initial spatial hypersurface Σ_0 (see Fig. 2a). Not just any embedding of Σ_0 with (γ_{ab}, K_{ab}) will specify initial data. GR describes *spacetimes*, so the time and spatial components cannot simply be decoupled. The pair (γ_{ab}, K_{ab}) has to satisfy the constraint equations, that follow from the Einstein equations, to be initial data [31, 32]. Finding solutions to the constraint equations and formulating initial data is a whole study by itself [33–37].



(a) We specify the initial data on the initial slice Σ_0. By evolving this in time we obtain a spacetime as an infinite stack of slices Σ_t.

(b) The coordinates x^a on different slices are identified by specifying a lapse N and shift N^a. Here, n^μ is the unit normal to the slice Σ_t.

Figure 2: In the ADM formalism, the spacetime is foliated by a family of time slices Σ_t.

For the BH binaries covered in this thesis, we shall use the conformal approach [21, 38]. This means we assume that the 3-metric γ_{ab} is related to some conformal background $\hat{\gamma}_{ab}$ by a conformal transformation ϕ, such that

$$\gamma_{ab} = \phi^4 \hat{\gamma}_{ab}. \tag{2.1}$$

Similarly, the extrinsic curvature K_{ab} will be split into its trace K and a conformally rescaled trace-free part $\hat{A}_{ab}$

$$K_{ab} = \phi^{-2}\hat{A}_{ab} + \frac{1}{3}\gamma_{ab}K. \tag{2.2}$$

In such a setting, the constraint equations take the following form in vacuum

$$8\hat{\nabla}^2\phi - \phi\hat{R} - \frac{2}{3}\phi^5 K^2 + \phi^{-7}\hat{A}_{ab}\hat{A}^{ab} = 0, \tag{2.3}$$

$$\hat{\nabla}_b\hat{A}^{ab} - \frac{2}{3}\phi^6\hat{\gamma}^{ab}\hat{\nabla}_b K = 0. \tag{2.4}$$

Here, $\hat{\nabla}_a$ denotes the covariant derivative, $\hat{R}$ the Ricci scalar and $\hat{\nabla}^2 = \hat{\gamma}^{ab}\hat{\nabla}_a\hat{\nabla}_b$ the Laplacian, which are all associated to the conformal background metric $\hat{\gamma}_{ab}$. Eq. (2.3) is known as the Hamiltonian constraint, and Eq. (2.4) is known as the momentum constraint. Note that $\hat{\gamma}_{ab}$ and K are freely specifiable. We assume our physical metric γ_{ab} to be conformally flat, i.e. $\hat{\gamma}_{ab} = \hat{f}_{ab}$ where $\hat{f}_{ab}$ is some flat, Euclidean 3-metric. Furthermore, we take a maximal slicing such that $K = 0$. These choices for $\hat{\gamma}_{ab}$ and K simplify the constraint Eqs. (2.3) and (2.4) to

$$\hat{\nabla}^2\phi = -\frac{1}{8}\phi^{-7}\hat{A}_{ab}\hat{A}^{ab}, \tag{2.5}$$

$$\hat{\nabla}_b\hat{A}^{ab} = 0. \tag{2.6}$$

An important consequence of this particular choice is that the momentum constraint (2.6) has become linear and decouples from the Hamiltonian constraint (2.5). Hence, we can find initial data by first solving equation (2.6) for $\hat{A}_{ab}$ and then the Poisson equation in (2.5) to determine the conformal factor ϕ, where the source term depends on $\hat{A}_{ab}$. Finally, all that is left is to determine the physical quantities (γ_{ab}, K_{ab}), using Eq. (2.1) and Eq. (2.2), respectively. In the context of the CLA, these equations commonly cannot be solved exactly and we have to rely on perturbative expansions to solve them order by order.

Some standard solutions to these equations are well known and often used as a template. When a system of BHs is initially at rest, Eq. (2.6) is trivially satisfied as $\hat{A}_{ab} = 0$ and Eq. (2.5) greatly simplifies. Two well-known solutions in this case are the Misner initial data [33] and Brill-Lindquist (BL) initial data [34]. The former can be used two describe BHs of the same mass, initially at rest. The latter is slightly more general and represents two BHs of different mass that have no initial momentum. The standard solution for two BHs with initial momentum is prescribed by Bowen-York (BY) initial data [35], which provides a solution for Eq. (2.6).

2.2 Regge-Wheeler perturbations

When we have constructed suitable initial data, we proceed with the next step: extracting the perturbations. In this step it is apparent why we call the approach the CLA as we expand everything in terms of some parameter ϵ related to the small separation of the BBH and sort all quantities in orders of ϵ, like Eq. (1.1).

In this thesis we restrict ourselves to a static, spherically symmetric Schwarzschild background. We can use these symmetries to our advantage and separate out the spherical components, which we will decompose in tensorial spherical harmonics, characterised by modes (ℓ, m) (see App. C). Since all the systems we will cover are axisymmetric, all non-vanishing perturbations satisfy $m = 0$. Consequently, for our purposes, we can use a basis of Legendre polynomials $P_\ell(\cos\theta)$ instead of spherical harmonics $Y^{\ell m}(\theta, \phi)$.[1]

[1]Using the basis $Y^{\ell 0}(\theta, \phi)$ instead of $P_\ell(\cos\theta)$ results in an additional factor $\sqrt{(2\ell - 1)/4\pi}$.

For the metric perturbations, it is customary to follow the conventions introduced by Regge and Wheeler in [39]. This results in two sets of perturbations: even and odd. Even parity modes change with sign $(-1)^\ell$ under parity transformations, while odd parity modes change with sign $(-1)^{\ell+1}$. We focus only on even perturbations, since the systems we study are symmetric under parity transformations. The metric perturbations in terms of even Regge-Wheeler quantities are given by:

$$^{(i)}g_{tt} = \left(1-\frac{2M}{r}\right)\sum_\ell {}^{(i)}H_0^{(\ell)}(r,t)P_\ell(\cos\theta), \tag{2.7}$$

$$^{(i)}g_{tr} = \sum_\ell {}^{(i)}H_1^{(\ell)}(r,t)P_\ell(\cos\theta), \tag{2.8}$$

$$^{(i)}g_{t\theta} = \sum_\ell {}^{(i)}h_0^{(\ell)}(r,t)\frac{\partial}{\partial\theta}P_\ell(\cos\theta), \tag{2.9}$$

$$^{(i)}g_{r\theta} = \sum_\ell {}^{(i)}h_1^{(\ell)}(r,t)\frac{\partial}{\partial\theta}P_\ell(\cos\theta), \tag{2.10}$$

$$^{(i)}g_{rr} = \left(1-\frac{2M}{r}\right)^{-1}\sum_\ell {}^{(i)}H_2^{(\ell)}(r,t)P_\ell(\cos\theta), \tag{2.11}$$

$$^{(i)}g_{\theta\theta} = r^2\sum_\ell \left[{}^{(i)}K^{(\ell)}(r,t) + {}^{(i)}G^{(\ell)}(r,t)\frac{\partial^2}{\partial\theta^2}\right]P_\ell(\cos\theta), \tag{2.12}$$

$$^{(i)}g_{\phi\phi} = r^2\sin^2\theta\sum_\ell \left[{}^{(i)}K^{(\ell)}(r,t) + {}^{(i)}G^{(\ell)}(r,t)\cot\theta\frac{\partial}{\partial\theta}\right]P_\ell(\cos\theta). \tag{2.13}$$

The other components vanish. In a similar fashion, the decomposition of the spatial metric γ_{ab} on Σ_0 is given by Eqs. (2.10)–(2.13). For convenience, we apply the same decomposition to the components of the extrinsic curvature K_{ab}. We denote its perturbations by

$$^{(i)}K_{r\theta} = \sum_\ell {}^{(i)}Kh_1^{(\ell)}(r,t)\frac{\partial}{\partial\theta}P_\ell(\cos\theta) \tag{2.14}$$

$$^{(i)}K_{rr} = \left(1-\frac{2M}{r}\right)^{-1}\sum_\ell {}^{(i)}KH_2^{(\ell)}(r,t)P_\ell(\cos\theta) \tag{2.15}$$

$$^{(i)}K_{\theta\theta} = r^2\sum_\ell \left[{}^{(i)}KK^{(\ell)}(r,t) + {}^{(i)}KG^{(\ell)}(r,t)\frac{\partial^2}{\partial\theta^2}\right]P_\ell(\cos\theta) \tag{2.16}$$

$$^{(i)}K_{\phi\phi} = r^2\sin^2\theta\sum_\ell \left[{}^{(i)}KK^{(\ell)}(r,t) + {}^{(i)}KG^{(\ell)}(r,t)\cot\theta\frac{\partial}{\partial\theta}\right]P_\ell(\cos\theta). \tag{2.17}$$

Now we have all the quantities we need to describe the system in a perturbative framework.

2.3 Gauge transformations

GR is a gauge theory in the sense that physical results do not depend on the chosen coordinates. In the context of perturbation theory, this means that the theory is invariant under infinitesimal coordinate transformations, that leave the background unchanged (see App. (A)). The expressions in Eqs. (2.7)–(2.13) and

Eqs. (2.14)–(2.17) are given in an arbitrary gauge. We still have the freedom to make a specific gauge choice that makes our calculations as convenient as possible, which will be especially important for the cumbersome expressions at second order.

Before we can apply gauge transformations to the perturbations, we have to reconstruct a 4-dimensional spacetime again from the 3-geometry. This is due to the fact that the choice for the embedding of Σ_0, with a corresponding choice of lapse N and shift N^a (see Fig. 2b), is a choice of coordinates in and of itself. To reconstruct the 4-dimensional metric $g_{\mu\nu}$ in a neighbourhood of Σ_0 from the initial data (γ_{ab}, K_{ab}), we perform a time expansion. This yields a local solution to the Einstein equations near Σ_0, which is all that we need as we are ultimately only interested in the initial data. This local solution $g_{\mu\nu}$ is described by the expansion

$$g_{\mu\nu} = g_{\mu\nu}|_{t=0} + t\,\partial_t g_{\mu\nu}|_{t=0} + \mathcal{O}(t^2).$$

Here, $g_{\mu\nu}|_{t=0}$ can be determined from the spatial metric γ_{ab} on Σ_0 by specifying a lapse N and shift vector N^a, which determines the embedding (see Fig. 2b). In the ADM formalism, a metric $g_{\mu\nu}$ is expressed in terms of a 3-metric γ_{ab} [31] as follows

$$g_{\mu\nu}\, dx^\mu dx^\nu = -N^2 dt^2 + \gamma_{ab}(dx^a + N^a dt)(dx^b + N^b dt). \tag{2.18}$$

At this point, we are free to specify the lapse and shift. We will choose them such that they vanish at all perturbative orders, i.e. ${}^{(i)}N = 0$ and ${}^{(i)}N^a = 0$ for all $i > 0$. In this case, the metric can be expanded as

$$g_{\mu\nu}\, dx^\mu dx^\nu = -{}^{(0)}N^2 dt^2 + {}^{(0)}\gamma_{ab}(dx^a + {}^{(0)}N^a dt)(dx^b + {}^{(0)}N^b dt) + \epsilon\, {}^{(1)}\gamma_{ab} dx^a dx^b + \epsilon^2\, {}^{(2)}\gamma_{ab} dx^a dx^b + \mathcal{O}(\epsilon^3).$$

From the form of the Schwarzschild metric in standard (t, r, θ, φ) coordinates, we can deduce that the shift vector ${}^{(0)}N^a$ also vanishes and the lapse function is given by ${}^{(0)}N = \sqrt{1-\frac{2M}{r}}$. Hence, we find that the future-directed unit normal to constant t-slices is given to all orders by

$$n^\mu = \left(\frac{1}{\sqrt{1-\frac{2M}{r}}}, 0, 0, 0\right), \qquad n_\mu = \left(-\sqrt{1-\frac{2M}{r}}, 0, 0, 0\right). \tag{2.19}$$

The extrinsic curvature K_{ab} is related to the 3-metric γ_{ab} via a Lie derivative with respect to the normal vector n^μ. Therefore, under assumption that the perturbative lapse and shift vanish, we have

$$\begin{aligned}
K_{ab} =& \frac{1}{2}\mathcal{L}_{\mathbf{n}}\gamma_{ab} \\
=& \frac{1}{2}\epsilon\mathcal{L}_{\mathbf{n}}\, {}^{(1)}\gamma_{ab} + \frac{1}{2}\epsilon^2\mathcal{L}_{\mathbf{n}}\, {}^{(2)}\gamma_{ab} + \mathcal{O}(\epsilon^3) \\
=& \frac{1}{2}\epsilon\left[n^\lambda\partial_\lambda\, {}^{(1)}\gamma_{ab} + 2\, {}^{(1)}\gamma_{\lambda(a}\partial_{b)}n^\lambda\right] \\
&+ \frac{1}{2}\epsilon^2\left[n^\lambda\partial_\lambda\, {}^{(2)}\gamma_{ab} + 2\, {}^{(2)}\gamma_{\lambda(a}\partial_{b)}n^\lambda\right] + \mathcal{O}(\epsilon^3) \\
=& \frac{1}{2}\frac{1}{\sqrt{1-\frac{2M}{r}}}\frac{\partial}{\partial t}\left[\epsilon\, {}^{(1)}\gamma_{ab} + \epsilon^2\, {}^{(2)}\gamma_{ab}\right] + \mathcal{O}(\epsilon^3),
\end{aligned}$$

where we used that ${}^{(0)}K_{ab} = 0$, since the Schwarzschild solution is stationary. In the last step, we observed that the symmetrisations ${}^{(i)}\gamma_{\lambda(a}\partial_{b)}n^\lambda$ vanish because ${}^{(i)}\gamma_{\mu\nu}$ only possesses spatial components, while n^μ only has a temporal one. Therefore, given our choice that the perturbative lapse and shift vanish, the following straightforward identification can be made

$$ {}^{(i)}K_{ab} = \tfrac{1}{2}\frac{1}{\sqrt{1-2M/r}}\frac{\partial}{\partial t}\,{}^{(i)}\gamma_{ab}. \tag{2.20} $$

Hence, the time expansion can be expressed as

$$ g_{\mu\nu} = g_{\mu\nu}|_{t=0} + 2t\sqrt{1-\frac{2M}{r}}\,K_{\mu\nu} + \mathcal{O}(t^2), \tag{2.21} $$

Now that we have reconstructed a proper spacetime metric $g_{\mu\nu}$, we can transform it under gauge transformations to switch from one gauge choice to another. Since we work in a second order framework, we have a first order transformation generated by ${}^{(1)}\xi^{\mu}$ and a second order transformation generated by ${}^{(2)}\xi^{\mu}$. Under a gauge transformation, the metric perturbations transform order by order as

$$ \begin{aligned} {}^{(0)}g'_{\mu\nu} &= {}^{(0)}g_{\mu\nu} \\ {}^{(1)}g'_{\mu\nu} &= {}^{(1)}g_{\mu\nu} + \mathcal{L}_{{}^{(1)}\xi}\,{}^{(0)}g_{\mu\nu} \\ {}^{(2)}g'_{\mu\nu} &= {}^{(2)}g_{\mu\nu} + \mathcal{L}_{{}^{(2)}\xi}\,{}^{(0)}g_{\mu\nu} + \mathcal{L}_{{}^{(1)}\xi}\,{}^{(1)}g_{\mu\nu} + \frac{1}{2}\mathcal{L}^2_{{}^{(1)}\xi}\,{}^{(0)}g_{\mu\nu}. \end{aligned} \tag{2.22} $$

The structure of these equations mandates a two step approach. First we fix the first order gauge by applying the transformations as a consequence of the generator ${}^{(1)}\xi^{\mu}$. We shall refer to this as the first order gauge transformation. Note that in our second order framework the first order gauge transformation must be carried out up to second order and, as a consequence, the second order perturbations in ${}^{(2)}g_{\mu\nu}$ also change. Now we proceed with the second order gauge transformation, which is the transformation generated by ${}^{(2)}\xi^{\mu}$, to fix the gauge at second order.

We have to be cautious with gauge choices in higher order perturbation theory. A second order gauge is not unique, since it depends explicitly on the particular gauge chosen at first order. Hence, we always have to be mindful of the choices made at first order. Similar problems apply to invariance. With the term "second order gauge invariance" we will refer to quantities that are invariant under the pure second order gauge transformation $\mathcal{L}_{{}^{(2)}\xi}\,{}^{(0)}g_{\mu\nu}$, while "first and second order invariance" pertains to invariance under the full transformation in Eq. (2.22) (also see App. C.1).

There are two gauge choices that are particularly important for our purposes. The first one, we have already encountered. This is choosing a gauge such that $H_0 = H_1 = h_0 = 0$, which amounts to choosing the perturbative lapse and shift to vanish. This allows for an easy identification between time derivatives of metric perturbations and perturbations of the extrinsic curvature, that is Eq. (2.20).

The other relevant choice is the RW gauge $h_0 = h_1 = G = 0$ (see App. C.1). This gauge choice is an integral part in the derivation for the master equation that governs the perturbations. The RW gauge also has the benefits that it fully fixes the gauge at the order where it is implemented and that the gauge invariant combinations in Eqs. (C.24)–(C.27) are simply equal to the corresponding perturbation in the RW gauge. Hence, we can easily recover the expressions in the RW gauge from any arbitrary gauge by taking its gauge invariant combination. We will also often use quantities in the RW gauge as a shorthand notation to represent the gauge invariant combination of perturbations (see Sec. 4.4), such as

$$ {}^{(1)}K^{\mathrm{RW}} \equiv {}^{(1)}K - \frac{2}{r}\left(1-\frac{2M}{r}\right)\left[{}^{(1)}h_1 - \frac{r^2}{2}\partial_r\,{}^{(1)}G\right], $$

for instance. Here ${}^{(1)}K^{\mathrm{RW}}$ is a perturbation in the RW gauge and the perturbations on the RHS are in an arbitrary gauge.

2.4 Evolving the System

Once we have obtained a set of gauge fixed initial perturbations, the final step is to evolve them in time to obtain the time development of the system. This can be accomplished by numerically integrating the master equation, describing the perturbations. For even RW perturbations the master equation is the Zerilli equation, which is an elegant way of recasting the Einstein equations in a Schrödinger-like equation [40].[2] We will derive this equation in detail in Sec. 4.4, using Zerilli's original derivation [40].[3]

As derived in App. B, the vacuum Einstein Equations take the following form when they are sorted order by order:

$$ {}^{(1)}R_{\mu\nu} = \delta R_{\mu\nu}[{}^{(1)}g] = 0, \tag{2.23} $$

$$ {}^{(2)}R_{\mu\nu} = \delta R_{\mu\nu}[{}^{(2)}g] = -\delta^2 R_{\mu\nu}[{}^{(1)}g, {}^{(1)}g], \tag{2.24} $$

where $\delta R_{\mu\nu}$ is linear in the perturbations and $\delta^2 R_{\mu\nu}$ is quadratic in the perturbations. Hence, solving the set of perturbative equations comes down to a step by step approach: first, we evolve the first order perturbations using Eq. (2.23), which can be reformulated as a Zerilli equation. Then, these perturbations are plugged in Eq. (2.24), where they will serve as a known source term that is quadratic in the first order perturbations. The evolution of the second order perturbations follows from the same Zerilli equation again, but now involving some known source term.

Therefore, the final analytical step before we have to resort to numerical methods is to recast our initial data in terms of a Zerilli equation and a corresponding master function $\psi^{(\ell)}$ that is a function of the even Regge-Wheeler perturbations for a particular ℓ-mode. At first order, the Einstein Eq. (2.23) can ultimately be rewritten as

$$ \frac{\partial^2\, {}^{(1)}\psi^{(\ell)}}{\partial r^{*2}} - \frac{\partial^2\, {}^{(1)}\psi^{(\ell)}}{\partial t^2} - V_\ell(r^*)\, {}^{(1)}\psi^{(\ell)} = 0. $$

At first order, we will use the Moncrief function that has the great advantage of being (first order) gauge invariant and being a function of only the 3-geometry [41]. This wavefunction takes the form

$$ {}^{(1)}\psi^{(\ell)} = \frac{2(r-2M)}{\ell(\ell+1)(\lambda r+3M)}\left[r\,{}^{(1)}{H_2}^{(\ell)} + 3r^2\frac{\partial\,{}^{(1)}G^{(\ell)}}{\partial r} - \frac{r-3M}{r-2M}\,{}^{(1)}K^{(\ell)} - r^2\frac{\partial\,{}^{(1)}K^{(\ell)}}{\partial r} - 6\,{}^{(1)}{h_1}^{(\ell)}\right] + \frac{r^2}{\lambda r+3M}\,{}^{(1)}K^{(\ell)}, $$

where the perturbations are in an arbitrary gauge. We could also have opted for the Zerilli wavefunction ${}^{(1)}\chi^{(\ell)}$ given by

$$ {}^{(1)}\chi^{(\ell)} = \frac{r-2M}{\lambda r+3M}\left[\frac{r^2}{r-2M}\frac{\partial\,{}^{(1)}K^{\mathrm{RW}}}{\partial t} - {}^{(1)}{H_1}^{\mathrm{RW}}\right], $$

where the perturbations are in the RW gauge and where we dropped some of the (ℓ) superscripts. This function satisfies the same equation and is related to the Moncrief function by $\partial_t\,{}^{(1)}\psi^{(\ell)} = {}^{(1)}\chi^{(\ell)}$. This easy identification between the two is only possible in the absence of a source term.

[2] In the case of odd perturbations, the linearised Einstein equations can also be recast in a Schrödinger-like equation called the Regge-Wheeler equation [39]. This derivation is far simpler than the one for even perturbations and inspired Zerilli's derivation.

[3] One could alternatively use Moncrief's alternative derivation [41] that yields the same differential equation, but with a slightly different wavefunction.

At second order, the Einstein equations in Eq. (2.24) yield a similar equation

$$\frac{\partial^2 \, {}^{(2)}\chi^{(\ell)}}{\partial r^{*2}} - \frac{\partial^2 \, {}^{(2)}\chi^{(\ell)}}{\partial t^2} - V_\ell(r^*) \, {}^{(2)}\chi^{(\ell)} = S({}^{(1)}\psi, {}^{(1)}\psi).$$

This is the same Zerilli equation, but now we also have an additional source term S. To derive the source term S, one needs to repeat the derivation for the Zerilli equation and carefully account for the quadratic terms as a result of $\delta^2 R_{\mu\nu}$. The source term introduces mixing between the different ℓ-modes. Again, we have to be careful at higher order: the source term S is not unique and depends on the choices we have made at first order, such as gauge choices. We will also use the Zerilli function ${}^{(2)}\chi^{(\ell)}$, instead of ${}^{(2)}\psi^{(\ell)}$, because this follows directly from our derivation and we cannot easily relate it to the Moncrief function anymore due to the source term.

The only remaining step is to numerically integrate these equations to obtain a time evolution of the perturbations. This is were the interesting physics arises.

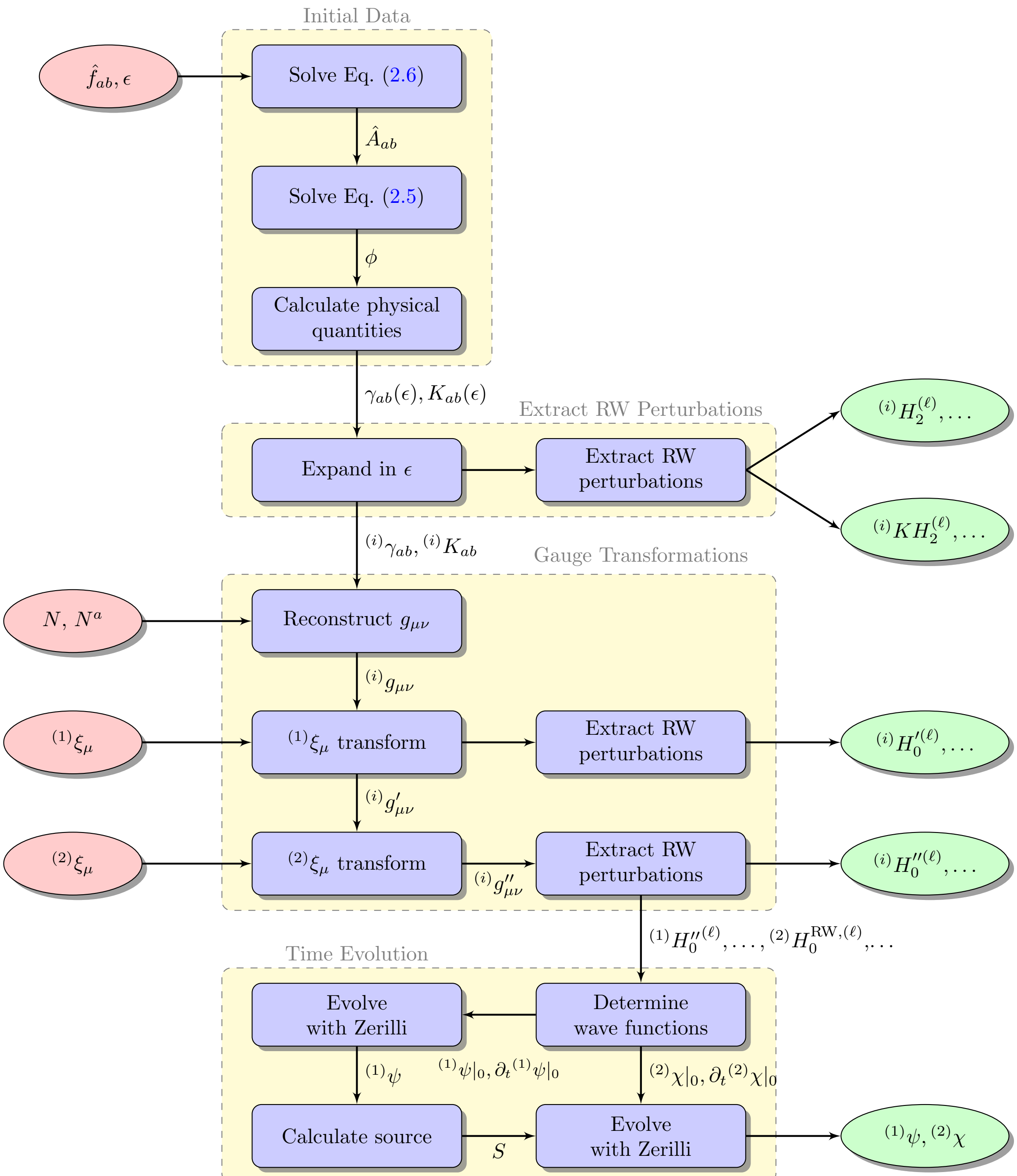


Figure 3: Flowchart of the steps involved in the CLA. Input is represented on the left in red, the involved steps are represented in blue and should be read from top to bottom following the arrows, and finally the outcomes are presented on the right side in green. The overall steps are grouped in yellow.

3 Static Black Holes

To illustrate how the CLA works in practice, we shall cover its easiest instance in the case of two BHs of the same mass, which are initially at rest. This system was covered in [5], where Price and Pullin first proposed the CLA. Since this section only serves as an example, we shall for the sake of simplicity only carry out the calculation up to first order. The intricacies of second order perturbation theory are left for the more extensive calculation in the next section.

We consider a system consisting of two black holes with equal bare mass m, initial coordinate separation L, and no instantaneous initial momentum. Before we continue we have to remark that L, as a coordinate distance, does not have a physical interpretation. It is customary to use the proper distance between the two apparent horizons of the BHs as a physical measure for the initial separation [29].

3.1 Formulating the Initial Data

The first step in applying the CLA to this system is to find suitable initial data to describe our system at $t = 0$. An important property of the initially static black holes is the time symmetry as a consequence of the absence of initial momentum. This symmetry allows us to easily use the Misner or BL initial data [34, 37]. The first CLA calculations have been carried out using Misner initial data [5, 16], but the calculation with BL initial data is more convenient to later generalise to initially moving BHs [19, 30]. Hence, we opt for the latter.

The family of BL initial data for two BHs of bare mass m_1 and m_2 is described by [34]

$$\gamma_{ab}^{\mathrm{BL}}\, dx^a dx^b = \phi_{\mathrm{BL}}^4 \hat{f}_{ab}\, dx^a dx^b = \phi_{\mathrm{BL}}^4 \left[dR^2 + R^2(d\theta^2 + \sin^2\theta d\varphi^2) \right], \tag{3.1}$$

where $\hat{f}_{ab}$ is the flat 3-metric, which we have expressed in spherical coordinates (R, θ, φ) and where we have the conformal factor

$$\phi_{\mathrm{BL}} \equiv 1 + \frac{m_1}{2\|\mathbf{R} - \mathbf{C}_1\|} + \frac{m_2}{2\|\mathbf{R} - \mathbf{C}_2\|}. \tag{3.2}$$

Here, $\|\ldots\|$ indicates the coordinate distance with respect to $\hat{f}_{ab}$, $\mathbf{R}$ denotes an arbitrary position in the conformal space and $\mathbf{C}_i$ is the position of the centre of the i-th BH. To fix the coordinates, we align the z-axis with the line connecting $\mathbf{C}_1$ to $\mathbf{C}_2$ (see Fig. 4). Now the BH centres are at $z = \pm L/2$. Since we are considering two BHs of the same mass, we set $m_1 = m_2 \equiv m$ in the remainder of this section. The total ADM mass $M$of the system is now given by $M = m_1 + m_2 = 2m$. Also note that ϕ_{BL} is singular at the two points $\mathbf{R} = \mathbf{R}_{1,2}$.

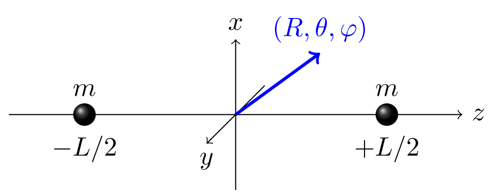


Figure 4: The coordinates (R, θ, φ), used in the conformal background $\hat{f}_{ab}$.

In its current coordinates (R, θ, φ), the comparison between the BL initial data and the Schwarzschild spacetime is not very evident. To aid this comparison we switch to a new radial coordinate given by

$$R = \tfrac{1}{4}(\sqrt{r} + \sqrt{r - 2M})^2,$$

and recognise that the conformal factor takes the form of a generating function for the Legendre polynomials. We find

$$\gamma_{ab}^{\mathrm{BL}}\, dx^a dx^b = \mathcal{F}_{\mathrm{BL}}^4(r,\theta;L)\left[\left(1-\frac{2M}{r}\right)^{-1} dr^2 + r^2(d\theta^2+\sin^2\theta\, d\varphi^2)\right], \tag{3.3}$$

where the conformal factor ϕ_{BL} has been rewritten to

$$\mathcal{F}_{\mathrm{BL}} = 1 + \left(1+\frac{M}{2R}\right)^{-1} \sum_{\ell=2,4,\ldots} \kappa_\ell(L)\left(\frac{M}{R}\right)^{\ell+1} P_\ell(\cos\theta). \tag{3.4}$$

The coefficients for the different Legendre polynomials are

$$\kappa_\ell(L) = \frac{1}{2}\left(\frac{L}{2M}\right)^{\ell}. \tag{3.5}$$

Observe the 3-metric in Eq. (3.3) takes the same form as a constant t-slice of the Schwarzschild spacetime modulo the conformal factor. This way, we have recast our initial data in a convenient form for the rest of the analysis.

3.2 Determining Regge-Wheeler Perturbations

The next step is actually implementing the CLA, i.e. putting the BHs close together and performing an expansion in the small initial separation L. Observe that in the limit $L \to 0$, which corresponds to $\kappa_\ell \to 0$, the conformal factor $\mathcal{F}$ approaches 1. Hence, our system reduces to a Schwarzschild time slice in this limit, making Schwarzschild perturbation theory the correct framework.

To apply perturbation theory, we note that the conformal factor $\mathcal{F}_{\mathrm{BL}}$ enters raised to the fourth power in the 3-metric. From Eq. (3.5), we deduce that in the small-L limit $1-\mathcal{F}_{\mathrm{BL}}$ consists solely of perturbations of order $L^2, L^4, \ldots$. Therefore, the metric perturbations scale with $L^2, L^4, L^6, \ldots$, since we have

$$\gamma_{ab}^{\mathrm{BL}}\, dx^a dx^b = \left(1 + 4\left(1+\frac{M}{2R}\right)^{-1} \sum_{\ell=2,4,\ldots} \kappa_\ell(L)\left(\frac{M}{R}\right)^{\ell+1} P_\ell(\cos\theta)\right)\left[\left(1-\frac{2M}{r}\right)^{-1} dr^2 + r^2 d\Omega^2\right],$$

where $d\Omega^2 = d\theta^2 + \sin^2\theta\, d\varphi^2$. The lowest appearing order, therefore, is L^2 and the next order L^4. Hence, we define our expansion parameter to be the dimensionless quantity $\epsilon \equiv L^2/M^2$.

Now that we have performed the expansion in small L, the next step is to extract the metric perturbations describing the system. In the perturbation theory pertaining to the Schwarzschild spacetime, it is customary to decompose the metric, using the notation of [39]. This was introduced in Eqs. (2.7)–(2.13). From Eq. (3.3), it is now easy to read off that the only non-vanishing perturbations are given by

$${}^{(1)}H_2{}^{(\ell=2)} = {}^{(1)}K_2{}^{(\ell=2)} = 4\kappa_2\left(1-\frac{2M}{R}\right)^{-1}\left(\frac{M}{R}\right)^3, \tag{3.6}$$

where we have included the expansion parameter ϵ in the expression for ${}^{(1)}H_2{}^{(\ell=2)}$. We will also do this for the remainder of this thesis to conform to the conventions used in the literature on the CLA.

3.3 Gauge transformations

At this point, we still have to deal with the gauge freedom of GR. The next step will be to fix the gauge to eliminate the extra degrees of freedom.

One aspect we have not covered so far is the time dependence of our system; we have only discussed the 3-geometry. Since our system is time symmetric, we have $\partial_t g_{\mu\nu} = 0$. This allows us to make an appropriate choice of lapse and shift such that

$$g_{\mu\nu}\, dx^\mu dx^\nu = -\left(1 - \frac{2M}{r}\right) dt^2 + \gamma_{ab}^{\text{BL}}\, dx^a dx^b + \mathcal{O}(t^2). \tag{3.7}$$

To attain this particular form of the spacetime metric $g_{\mu\nu}$, we have essentially made the gauge choice ${}^{(1)}H_1 = {}^{(1)}h_0 = {}^{(1)}h_1 = 0$. This amounts to choosing a lapse ${}^{(0)}N = \sqrt{1-2M/r}$ and shift ${}^{(0)}N^a = 0$ for the background and choosing the perturbative lapse and shift to vanish at all orders.

To attain this gauge we do not have to perform any complicated gauge transformations. In fact, nothing really changes for the 3-geometry specified above and ${}^{(1)}H_2{}^{(\ell=2)}$ and ${}^{(1)}K^{(\ell=2)}$ as given in Eq. (3.6) are still the only non-vanishing perturbations after fixing the gauge.

Another important gauge choice is the Regge-Wheeler gauge: ${}^{(1)}G = {}^{(1)}h_0 = {}^{(1)}h_1 = 0$ for even perturbations. Perturbations in the RW-gauge can be viewed as gauge invariant combination of perturbations in any arbitrary gauge (see Appendix C.1). Since our system already satisfies this condition we simply have

$${}^{(1)}H_2{}^{\text{RW},(\ell=2)} = {}^{(1)}K_2{}^{\text{RW},(\ell=2)} = 2\kappa_2 \left(1 - \frac{2M}{R}\right)^{-1} \left(\frac{2M}{R}\right)^3. \tag{3.8}$$

By specifying our system in the RW-gauge we have fully gauge fixed our system at first order [42], so that all degrees of freedom pertaining to the gauge freedom have been eliminated.

3.4 Zerilli Equation

The final step is to evolve the initial data in time. The even Regge-Wheeler perturbations are governed by the Zerilli equation [40]. A longer exposition and full derivation of this equation can be found in Sec. 4.4. In short, the initial data can be evolved using

$$\frac{\partial^2\, {}^{(1)}\psi^{(\ell=2)}}{\partial r^{*2}} - \frac{\partial^2\, {}^{(1)}\psi^{(\ell=2)}}{\partial t^2} - V_2(r^*)\, {}^{(1)}\psi^{(\ell=2)} = 0,$$

where the potential $V_\ell(r^*)$ for $\ell = 2$ is given by

$$V_2(r^*) = 2\left(1 - \frac{2M}{r}\right) \frac{4r^2(3r+3M) + 9M^2(2r+M)}{r^3(2r+3M)^2},$$

and where the Moncrief-Zerilli function is the following gauge invariant combination of perturbations

$${}^{(1)}\psi^{(\ell=2)} = \frac{r-2M}{3(2r+3M)}\left[r\,{}^{(1)}H_2{}^{(\ell=2)} + 3r^2 \frac{\partial^{(1)}G^{(\ell=2)}}{\partial r} - r^2 \frac{\partial^{(1)}K^{(\ell=2)}}{\partial r} - 6\,{}^{(1)}h_1{}^{(\ell=2)}\right] - \frac{r}{3}\,{}^{(1)}K^{(\ell=2)}.$$

Now we supply the initial function ${}^{(1)}\psi^{(\ell=2)}|_{t=0}$ in terms of the initial perturbations into some solver to numerically integrate the Zerilli equation. We also have to supply the time derivative $\partial_t\, {}^{(1)}\psi^{(\ell=2)}|_{t=0}$ as initial data, but this simply vanishes as a consequence of the time symmetry of the initial data.

4 Head-on collision

As we have seen in the previous section, a system of two initially static BHs of the same mass, represented by BL initial data, can quite easily be described with the CLA due to its convenient analytical form. However, from an astrophysical perspective, two static BHs are not a very realistic representation of reality, so we generalise this system by giving initial momentum to both BHs. To keep expressions somewhat manageable, which will be especially important for the second order calculations, we will opt for a system with high degree of symmetry.

In this section, we will apply the CLA to two BHs with the same bare mass m, that are in a head-on collision with the same, opposing initial momentum $\mathbf{P}$ (see Fig. 5). The BHs have an initial coordinate separation L. Furthermore, we also make the simplification that P is of the same order as L. This implies that terms with a factor L^2, P^2 and PL are all of the same order, which will simply be denoted as $\mathcal{O}(L^2)$. Since all lowest order perturbations are of order $\mathcal{O}(L^2)$, we will refer to these terms as being first order. The second order terms turn out to be terms like $L^4, L^2P^2, \ldots$, which are of order $\mathcal{O}(L^4)$.

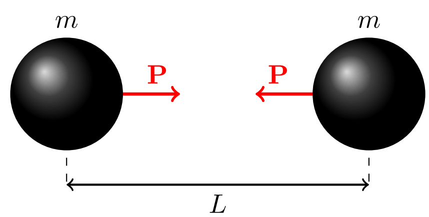


Figure 5: Schematic overview of the considered system of two BHs in a head-on collision.

We have followed the approach taken in [25] to analyse this system. As we will see, our calculations agree at first order, but at second order we run into some discrepancies. Throughout this section we will comment on the differences and try to relate our expressions to [25].

4.1 Formulating the Initial Data

The first step in setting up the CLA for this system is constructing the initial data. This requires specifying a spatial 3-metric γ_{ab} and extrinsic curvature K_{ab} on some initial spatial hypersurface Σ_0, such that the constraint equations of GR are satisfied. Like we discussed in Sec. 2, we will use the conformal approach and start from some conformal 3-metric $\gamma_{ab} = \phi^4 \hat{f}_{ab}$, where $\hat{f}_{ab}$ is a flat metric that we will express in spherical coordinates (R, θ, φ) as

$$\hat{f}_{ab} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & R^2 & 0 \\ 0 & 0 & R^2 \sin^2\theta \end{pmatrix}. \tag{4.1}$$

Now we want to determine the conformal, trace-free extrinsic curvature $\hat{A}_{ab}$ and conformal factor ϕ that satisfy the constraint equations. First, we need to solve the momentum constraint Eq. (2.6). The solution for a single boosted BH with its centre at position $\mathbf{C}$ and momentum $\mathbf{P}$ is given by the BY solution [35], which is described by

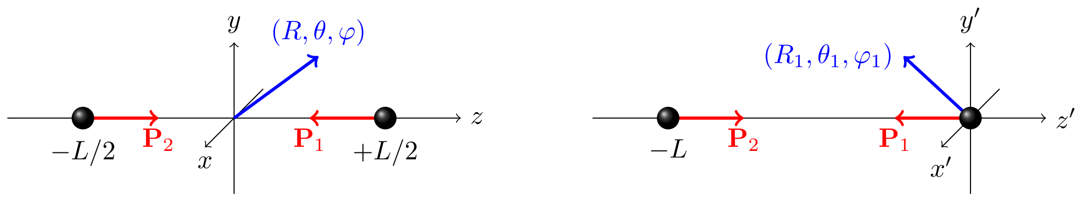
$$\hat{A}_{ab}^{\mathbf{CP}} = \frac{3}{2R_{\mathbf{C}}^2}\left[2P_{(a}n_{b)} - (\hat{f}_{ab} - n_a n_b)P^c n_c\right], \tag{4.2}$$

where $R_{\mathbf{C}} = \|\mathbf{R} - \mathbf{C}\|$ is the coordinate distance between the centre of the BH and an arbitrary point with respect to the flat metric $\hat{f}_{ab}$. Furthermore, P_a is the momentum vector and n_a is a radial unit normal vector that is perpendicular to a sphere of constant radius. This solution describes a single boosted BH. However, we are interested in two BHs in a head-on collision. Since the momentum constraint Eq. (2.6) is linear, this can easily be adjusted by taking a superposition of two solutions for $\hat{A}_{ab}$. Therefore, in the case of two BHs at position $\mathbf{C}_1$ and $\mathbf{C}_2$ with momentum $\mathbf{P}_1$ and $\mathbf{P}_2$, respectively, the solution for the traceless, conformal extrinsic curvature $\hat{A}_{ab}$ is given by

$$\hat{A}_{ab} = \hat{A}_{ab}^{\mathbf{C}_1\mathbf{P}_1} + \hat{A}_{ab}^{\mathbf{C}_2\mathbf{P}_2}. \tag{4.3}$$

The next step would be to find the conformal factor ϕ. The Poisson equation resulting from the Hamiltonian constraint Eq. (2.5) does not admit an analytical solution in closed form, in most cases. Hence, we will solve it perturbatively in the regime where the initial separation and momentum are small.

The first step for solving the Poisson equation in Eq. (2.5) perturbatively is expanding the extrinsic curvature in terms of the order parameter L. To accomplish this, we switch to a more convenient basis by centring the origin at one of the BHs. In the original coordinate system the first BH was located at position $(x, y, z) = (0, 0, L/2)$ and in the new centred coordinates it is located at $(x', y', z') = (0, 0, 0)$ (see Fig. 6). The second BH is translated from $(x, y, z) = (0, 0, -L/2)$ to $(x', y', z') = (0, 0, -L)$.



(a) Original coordinate system (b) Translated coordinate system

Figure 6: We transform the original coordinates (R, θ, ϕ) to (R_1, θ_1, ϕ_1) by repositioning the origin of the new coordinates in the centre of the right BH.

After translating the Cartesian coordinates, the spherical coordinates (R, θ, φ) also have to be reformulated as $(R_1, \theta_1, \varphi_1)$ centred at one BH. In terms of the old spherical coordinates, the new spherical coordinate system becomes

$$R_1 = \sqrt{x'^2 + y'^2 + z'^2} = \sqrt{R^2 + L^2/4 - RL\cos\theta}, \tag{4.4}$$

$$\cos\theta_1 = \frac{z'}{R_1} = \frac{R\cos\theta - L/2}{\sqrt{R^2 + L^2/4 - RL\cos\theta}}, \tag{4.5}$$

$$\varphi_1 = \operatorname{sgn}(y')\frac{x'}{\sqrt{x'^2 + y'^2}} = \varphi. \tag{4.6}$$

The vectors $\mathbf{n}_1$ and $\mathbf{P}_1$ can now be expressed in a covariant basis as

$$\mathbf{n}_1 = dR_1 = \frac{2R - L\cos\theta}{2R_1}\, dR + \frac{RL\sin\theta}{2R_1}\, d\theta, \tag{4.7}$$

$$\mathbf{P}_1 = -P\, dz' = -P\left[\cos\theta\, dR - R\sin\theta\, d\theta\right]. \tag{4.8}$$

Now we have all quantities required in order to calculate $\hat{A}_{ab}^{\mathbf{C}_1\mathbf{P}_1}$ in terms of the coordinates (R, θ, φ). For the full expression for $\hat{A}_{ab}^{\mathbf{C}_1\mathbf{P}_1}$ we refer to the `HeadOnCollision.nb` notebook [43]. To calculate $\hat{A}_{ab}^{\mathbf{C}_2\mathbf{P}_2}$ we apply a similar approach, but now the coordinates will be centred at the other BH. This will result in some sign changes, e.g. $R_2 = \sqrt{R^2 + L^2/4 + RL\cos\theta}$. In this case, the vectors become

$$\mathbf{n}_2 = dR_2 = \frac{2R + L\cos\theta}{2R_2}\, dR - \frac{RL\sin\theta}{2R_2}\, d\theta, \tag{4.9}$$

$$\mathbf{P}_1 = P\, dz' = P\left[\cos\theta\, dR - R\sin\theta\, d\theta\right], \tag{4.10}$$

and we find an expression for $\hat{A}_{ab}^{\mathbf{C}_2\mathbf{P}_2}$ very similar to $\hat{A}_{ab}^{\mathbf{C}_1\mathbf{P}_1}$, except for some different signs. The full expression for the total $\hat{A}_{ab} = \hat{A}_{ab}^{\mathbf{C}_1\mathbf{P}_1} + \hat{A}_{ab}^{\mathbf{C}_2\mathbf{P}_2}$ is rather cumbersome. At this point, we will resort to perturbation theory and expand $\hat{A}_{ab}$ in terms of the L and P. Recall that L and P were assumed to be of similar order. For the conformal extrinsic curvature, first order terms scale with PL and second order terms scale with PL^3. This expansion yields

$$\hat{A}_{ab} = \frac{3LP}{2R^3}\begin{pmatrix} -4\cos^2\theta & 0 & 0 \\ 0 & R^2[1+\cos^2\theta] & 0 \\ 0 & 0 & R^2[-1+4\cos^2\theta - 3\cos^4\theta] \end{pmatrix}$$
$$- \frac{3L^3P}{16R^5}\begin{pmatrix} 2\left[1 - 18\cos^2\theta + 25\cos^4\theta\right] & 4R\left[-1+5\cos\theta^2\right]\cos\theta\sin\theta & 0 \\ 4R\left[-1+5\cos\theta^2\right]\cos\theta\sin\theta & R^2\left[1+6\cos^2\theta - 15\cos^4\theta\right] & 0 \\ 0 & 0 & R^2\left[-3+33\cos^2\theta - 65\cos^4\theta + 35\cos^6\theta\right] \end{pmatrix}.$$

This agrees with Eq. (4) in [25].

The following step is to determine conformal factor ϕ from the Hamiltonian constraint Eq. (2.5), where the contraction $\hat{A}_{ab}\hat{A}^{ab}$ enters as a source term. In the case of vanishing extrinsic curvature, i.e. for two momentarily static BHs, we have already encountered the solution. This is the BL initial data with its conformal factor given in Eq. (3.2). Again we take $m_1 = m_2 = m$.

In order to account for the BHs' boosts, we will add a regularising term ϕ_{reg} to the Brill-Linquist solution ϕ_{BL}, such that

$$\phi = \phi_{\text{reg}} + \phi_{\text{BL}}. \tag{4.11}$$

This regularising term has to solve the equation

$$\hat{\nabla}^2\phi_{\text{reg}} = -\frac{1}{8}\frac{\hat{K}_{ab}\hat{K}^{ab}}{(\phi_{\text{BL}} + \phi_{\text{reg}})^7}, \tag{4.12}$$

with the boundary conditions that ϕ_{reg} is regular at both $\mathbf{R} = \mathbf{C}_i$ and approaches zero at infinity. We will solve Eq. (4.12) perturbatively for ϕ_{reg} up to second order. The conformal extrinsic curvature is of order PL, so the source term will be of second order P^2L^2. Hence, we make the ansatz

$$\phi_{\text{reg}} = P^2L^{2\,(2)}\phi + \mathcal{O}(L^6). \tag{4.13}$$

In order to find a solution for ${}^{(2)}\phi$, we expand the source term in Eq. (4.12) up to second order. This expansion results in

$$\begin{aligned}\hat{K}_{ab}\hat{K}^{ab} &= \frac{117L^2P^2\cos^4(\theta)}{2R^6} - \frac{9L^2P^2\cos^2(\theta)}{R^6} + \frac{9L^2P^2}{2R^6} + \mathcal{O}\left(L^6\right) \\ &= \frac{9L^2P^2}{2R^6}(1 - 2\cos^2\theta + 13\cos^4\theta) + \mathcal{O}\left(L^6\right).\end{aligned} \tag{4.14}$$

Furthermore, we only take the leading order into account in the denominator of Eq. (4.12). In other words, we approximate

$$\phi_{\rm BL} + \phi_{\rm reg} = 1 + \frac{M}{2R} + \mathcal{O}(L^2).$$

Here, the mass M is the ADM mass related to the bare mass m by the correction

$$2m = M + P^2 L^2 \, {}^{(2)}M + \mathcal{O}(L^6),$$

where ${}^{(2)}M$ is some correction coefficient. Since this correction only results in changes of the irrelevant $\ell = 0$ modes at second order, which are non-radiative, we simply ignore them and replace $2m$ by M and vice versa [25]. We find that ${}^{(2)}\phi$ should satisfy the following equation

$$P^2 L^2 \hat{\nabla}^2 \, {}^{(2)}\phi = {}^{(2)}S \equiv -72 P^2 L^2 \frac{R(1 - 2\cos^2\theta + 13\cos^4\theta)}{(2R+M)^7}. \tag{4.15}$$

We impose the boundary conditions that ${}^{(2)}\phi \to 0$ as $R \to \infty$. This problem can be further simplified by decomposing the source term ${}^{(2)}S$ into its respective multipoles. In this multipole expansion, it takes the form

$${}^{(2)}S = \sum_\ell {}^{(2)}S^{(\ell)} P_\ell(\cos\theta), \tag{4.16}$$

where $P_\ell(\cos\theta)$ are the Legendre polynomials again. The multipoles can be calculated from the orthogonality relation satisfied by the Legendre polynomials. This yields the decomposition

$$\begin{aligned} {}^{(2)}S^{(\ell=0)} &= -\frac{1056}{5} \frac{P^2 L^2 R}{(2R+M)^7}, \\ {}^{(2)}S^{(\ell=2)} &= -\frac{3072}{7} \frac{P^2 L^2 R}{(2R+M)^7}, \\ {}^{(2)}S^{(\ell=4)} &= -\frac{7488}{35} \frac{P^2 L^2 R}{(2R+M)^7}, \end{aligned} \tag{4.17}$$

and all other ${}^{(2)}S^{(\ell)}$ vanish. We also decompose ${}^{(2)}\phi$ in multipoles as

$${}^{(2)}\phi = {}^{(2)}\phi^{(\ell=0)} P_0(\cos\theta) + {}^{(2)}\phi^{(\ell=2)} P_2(\cos\theta) + {}^{(2)}\phi^{(\ell=4)} P_4(\cos\theta). \tag{4.18}$$

The Poisson equation in Eq. (4.15) can be solved by solving the resulting equations for each multipole separately, since the Legendre polynomials are eigenfunctions of the Laplacian. For each ℓ the following equation must be satisfied

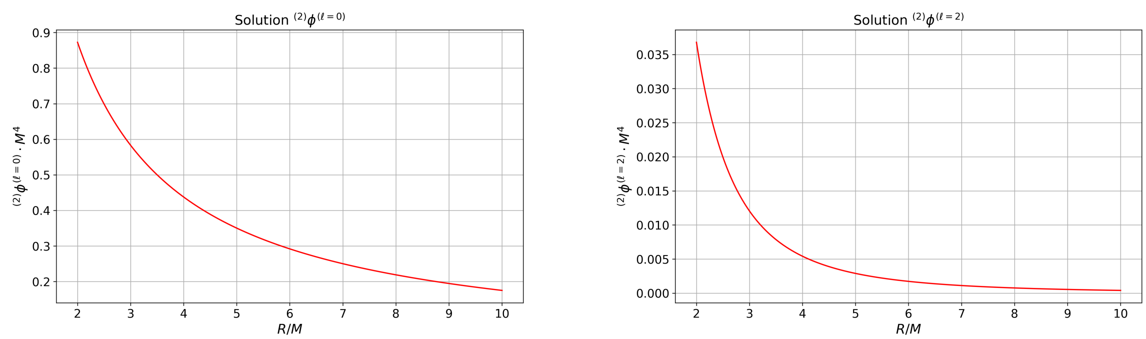
$$P^2 L^2 \hat{\nabla}^2 \left({}^{(2)}\phi^{(\ell)} P_\ell(\cos\theta) \right) = {}^{(2)}S^{(\ell)} P_\ell(\cos\theta). \tag{4.19}$$

Writing out the Laplacian for the flat background metric $\hat{f}_{ab}$ in spherical coordinates (R, θ, φ), we obtain

$$\frac{P_\ell(\cos\theta)}{R} \frac{\partial}{\partial R}\left(R^2 \frac{\partial \, {}^{(2)}\phi^{(\ell)}}{\partial R} \right) + \frac{{}^{(2)}\phi^{(\ell)}}{R^2 \sin\theta} \frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial P_\ell(\cos\theta)}{\partial\theta} \right) + \frac{{}^{(2)}\phi^{(\ell)}}{R^2 \sin^2\theta} \frac{\partial^2 P_\ell(\cos\theta)}{\partial\varphi^2} = \frac{{}^{(2)}S^{(\ell)} P_\ell(\cos\theta)}{P^2 L^2}.$$

Multiplying this equation by ${}^{(2)}\phi^{(\ell)} P_\ell(\cos\theta)$ and dividing it by R^2, yields

$$\frac{1}{{}^{(2)}\phi^{(\ell)}} \frac{\partial}{\partial R}\left(R^2 \frac{\partial \, {}^{(2)}\phi^{(\ell)}}{\partial R} \right) + \underbrace{\frac{1}{P_\ell \sin\theta} \frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial P_\ell}{\partial\theta} \right) + \frac{1}{P_\ell \sin^2\theta} \frac{\partial^2 P_\ell}{\partial\varphi^2}}_{-\ell(\ell+1)} = R^2 \frac{{}^{(2)}S^{(\ell)}}{P^2 L^2 \, {}^{(2)}\phi^{(\ell)}}.$$



(a) Plot of ${}^{(2)}\phi^{(\ell=0)}$ with $q_0 = 0.219 \cdot 2^3/M^3$.

(b) Plot of ${}^{(2)}\phi^{(\ell=2)}$ with $q_2 = 0.224 \cdot 2/M$.

Figure 7: Plots of the components of ${}^{(2)}\phi$ as a function of R. For convenience, we have plotted the functions for $M = 1$.

Here, we recognise that the angular part of the Laplace equation equals $-\ell(\ell+1)$. Therefore, the radial part results in a Riedel Equation for each multipole:

$$\begin{aligned}
\frac{\partial}{\partial R}\left(R^2 \frac{\partial^{(2)}\phi^{(\ell=0)}}{\partial R}\right) &= -\frac{1056}{5}\frac{R^3}{(2R+M)^7},\\
\frac{\partial}{\partial R}\left(R^2 \frac{\partial^{(2)}\phi^{(\ell=2)}}{\partial R}\right) - 6\ {}^{(2)}\phi^{(\ell=2)} &= -\frac{3072}{7}\frac{R^3}{(2R+M)^7},\\
\frac{\partial}{\partial R}\left(R^2 \frac{\partial^{(2)}\phi^{(\ell=4)}}{\partial R}\right) - 20\ {}^{(2)}\phi^{(\ell=4)} &= -\frac{7488}{35}\frac{R^3}{(2R+M)^7}.
\end{aligned}$$

The solutions to this ordinary differential equations are

$$ {}^{(2)}\phi^{(\ell=0)} = \frac{q_0}{R} - \frac{11\left(M^2 + 8MR + 20R^2\right)}{50R(M+2R)^5}, \tag{4.20}$$

$$ {}^{(2)}\phi^{(\ell=2)} = \frac{q_2}{R^3} - \frac{8\left(M^4 + 10M^3R + 40M^2R^2 + 80MR^3 + 80R^4\right)}{35R^3(M+2R)^5}. \tag{4.21}$$

We have not presented ${}^{(2)}\phi^{(\ell=4)}$ here in print, because of its lengthy expression, but it can be found in `HeadOnCollision.nb` [43]. The coefficients q_0 and q_2 are integration constants that are determined by the boundary condition that $\phi_{\rm reg}$ should be regular at both $\mathbf{R} = \mathbf{C}_i$. According to [25], the values are $q_0 = 0.219/m^3$ and $q_2 = 0.224/m$, which also agree with [44]. The solutions for ${}^{(2)}\phi^{(\ell=0)}$ and ${}^{(2)}\phi^{(\ell=2)}$ as a function of R have been plotted in Fig. 7.

At this point, we have perturbatively constructed the conformal factor ϕ and have thus found a solution to the initial value Eqs. (2.4) and (2.3). The conformal factor ϕ and conformal extrinsic curvature $\hat{A}_{ab}$ can now be substituted in Eqs. (2.1) and (2.2) to determine the physical 3-metric γ_{ab} and physical extrinsic curvature K_{ab}. So far, our calculations are in agreement with [25].

4.2 Determining Regge-Wheeler perturbations

Now that we have constructed initial data for our system, the CLA can be applied and we will treat our system as a deformation of a Schwarzschild BH. To facilitate comparison to the background, we make the following change of coordinates to switch from the flat radial coordinate R to the Schwarzschild radial coordinate r. This transformation is given by

$$R = \tfrac{1}{4}(\sqrt{r} + \sqrt{r-2M}). \tag{4.22}$$

Note that this transformation satisfies

$$\frac{\partial R}{\partial r} = \frac{R}{r}\frac{1}{\sqrt{1-\frac{2M}{r}}}.$$

Upon switching from the coordinates $x^a = (R, \theta, \varphi)$ to $y^a = (r, \theta, \varphi)$, the physical metric γ_{ab} is given by

$$\gamma_{ab}(y) = \frac{\partial x^i}{\partial y^a}\frac{\partial x^j}{\partial y^b}\phi^4 \hat{f}_{ij}(x). \tag{4.23}$$

To extract the metric perturbations, we use the same conventions as introduced in Eqs. (2.11)–(2.13). The Regge-Wheeler quantities can be deduced from Eq. (4.23). To this end, we proceed by also decomposing $\phi_{\rm BL}$ in Legendre polynomials to find the following multipoles

$$\phi_{\rm BL}^{(\ell=0)} = 1 + \frac{M}{2R} = 1 + \frac{2M}{\left(\sqrt{r-2M}+\sqrt{r}\right)^2}, \tag{4.24}$$

$$\phi_{\rm BL}^{(\ell=2)} = \frac{L^2 M}{8R^3} = \frac{8L^2 M}{\left(\sqrt{r-2M}+\sqrt{r}\right)^6}, \tag{4.25}$$

$$\phi_{\rm BL}^{(\ell=4)} = \frac{L^4 M}{32R^5} = \frac{32L^4 M}{\left(\sqrt{r-2M}+\sqrt{r}\right)^{10}}. \tag{4.26}$$

Since the initial geometry is conformally flat, the only non-vanishing metric perturbations are H_2 and K. The corresponding components of the 3-metric in Eq. (4.23) are given by

$$\gamma_{rr} = \left(\frac{\partial R}{\partial r}\right)^2 \phi^4 \hat{f}_{rr} = \left(\frac{R}{r}\right)^2 \frac{1}{1-2M/r}\phi^4, \tag{4.27}$$

$$\gamma_{\theta\theta} = \phi^4 \hat{f}_{\theta\theta} = \phi^4 R^2. \tag{4.28}$$

Combining this with Eq. (2.11) and (2.12), this implies that H_2 and K are equal, since they satisfy

$$H_2^{(\ell)} = \left(1 - \frac{2M}{r}\right)\gamma_{rr} = \left(\frac{R}{r}\right)^2 \phi^4 = \frac{1}{r^2}\gamma_{\theta\theta} = K^{(\ell)}.$$

Thus far, we have encountered quantities that featured $\ell = 0$, $\ell = 2$ and $\ell = 4$ modes. Since the $\ell = 2$ multipole is dominant and the $\ell = 0$ and $\ell = 2$ modes contribute to the corresponding source term at second order, we will only consider the $\ell = 0$ and $\ell = 2$ modes from this point onwards. The monopole and quadrupole moments follow from Eq. (4.27) or Eq. (4.28) by applying the orthogonality relations. The $\ell = 0$

contributions only start appearing at second order, where we find

$$
\begin{aligned}
{}^{(2)}{H_2}^{(\ell=0)} = {}^{(2)}K^{(\ell=0)} = &\frac{128L^4\left(15M^2r^2 + 30\left(r^4 - \sqrt{r^7(r-2M)}\right) + 30M\left(\sqrt{r^5(r-2M)} - 2r^3\right)\right)}{25M^2r^3\left(\sqrt{r-2M}+\sqrt{r}\right)^6} \\
&+ L^2P^2\Bigg(\frac{800q_0\left(M^4\left(\sqrt{r^5(r-2M)} + 5r^3\right) - 6M^3\sqrt{r^7(r-2M)} - 10M^3r^4 + 4M^2\sqrt{r^9(r-2M)} + 4M^2r^5\right)}{25M^2r^3\left(\sqrt{r-2M}+\sqrt{r}\right)^6} \\
&+ \frac{8\left(-11M^4 + 88M^3r + 33M^3\sqrt{r(r-2M)} - 55M^2\sqrt{r^3(r-2M)} - 55M^2r^2\right)}{25M^2r^3\left(\sqrt{r-2M}+\sqrt{r}\right)^6}\Bigg).
\end{aligned}
$$

The $\ell = 2$ multipole possesses both first and second order contributions. At first order, we have

$$
{}^{(1)}{H_2}^{(\ell=2)} = {}^{(1)}K^{(\ell=2)} = \frac{16L^2M}{\sqrt{r}\left(\sqrt{r-2M}+\sqrt{r}\right)^5},
$$

and at second order we have

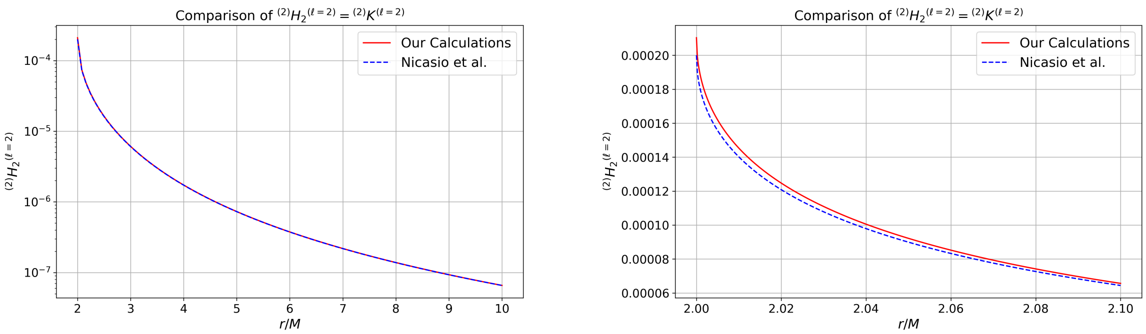
$$
\begin{aligned}
{}^{(2)}{H_2}^{(\ell=2)} = {}^{(2)}K^{(\ell=2)} = &\frac{192L^4M^2}{7r\left(\sqrt{r-2M}+\sqrt{r}\right)^{10}} \\
&+ L^2P^2\Bigg[\frac{640q_2\left(28M^2\sqrt{r^5(r-2M)} + 140M^2r^3 + 112\sqrt{r^9(r-2M)} - 168M\sqrt{r^7(r-2M)} - 280Mr^4 + 1120r^5\right)}{35r^3\left(\sqrt{r-2M}+\sqrt{r}\right)^{10}} \\
&+ \frac{64\left(-16M^4 + 80M^3\left(\sqrt{r(r-2M)} + 5r\right) - 640M^2\sqrt{r^3(r-2M)} - 1600M^2r^2 - 640\sqrt{r^7(r-2M)}\right)}{35r^3\left(\sqrt{r-2M}+\sqrt{r}\right)^{10}} \\
&+ \frac{64\left(1280M\sqrt{r^5(r-2M)} + 1920Mr^3 - 640r^4\right)}{35r^3\left(\sqrt{r-2M}+\sqrt{r}\right)^{10}}\Bigg].
\end{aligned}
$$

These expressions differ significantly from those found in the literature in [25]. In their work, Nicasio *et al.* found

$$
\begin{aligned}
H_2^{(\ell=2)} \quad = \quad K^{(\ell=2)} = &\frac{16ML^2}{\sqrt{r}(\sqrt{r}+\sqrt{r-2M})^5} + \frac{192M^2L^4}{7r(\sqrt{r}+\sqrt{r-2M})^{10}} + \frac{128L^2P^2q_2}{\sqrt{r}(\sqrt{r}+\sqrt{r-2M})^5} \\
&- \frac{256L^2P^2[12r^2 - 9rM + M^2 + (8r-3M)\sqrt{r}\sqrt{r-2M}]}{35r^3(\sqrt{r}+\sqrt{r-2M})^6}.
\end{aligned} \tag{4.29}
$$

At first order, the calculations agree and we find the same ${}^{(1)}{H_2}^{(\ell=2)}$. At second order, however, the L^2P^2 term in our calculations is more complicated than the term in [25]. Both expressions for L^2P^2 exhibit the same scaling behaviour at infinity. In both works, the q_2-term scales with $\mathcal{O}(r^{-3})$ and the remaining term scales with $\mathcal{O}(r^{-4})$. At the horizon $r = 2M$, the expressions also show similar behaviour. Their leading order term of order $\mathcal{O}([r-2M]^0)$ is even the same. When we plot both expressions (see Fig. 8), it becomes clear that the expression in our calculations includes some additional contributions near the horizon.

The initial configuration of colliding BHs is not static and as such there are also non-vanishing contributions for the extrinsic curvature. We apply the same decomposition to them as for the metric perturbations, i.e.



(a) Plot for large values of r/M.

(b) Plot for small values of r/M near the horizon.

Figure 8: Comparison of $H_2^{(\ell=2)} = K^{(\ell=2)}$ in our calculations to the expressions from [25]. Graphs have been plotted for $M = 1$, $L = 0.01$, $P = 0.01$ and $q_2 = 0.224 \cdot 2/M$.

Eqs. (2.15)–(2.17). The physical extrinsic curvature, expressed in the new Schwarzschild coordinates, follows from

$$K_{ab}(y) = \frac{\partial x^i}{\partial y^a}\frac{\partial x^j}{\partial y^b}\phi^{-2}\hat{K}_{ij}(x). \tag{4.30}$$

Again, we apply the orthogonality of Legendre polynomials in order to determine the monopole and quadrupole contributions. We have two non-vanishing $\ell = 0$ modes at first order given by

$$ {}^{(1)}KH_2{}^{(\ell=0)} = -\frac{2LP}{r^3}, \tag{4.31}$$

$$ {}^{(1)}KK^{(\ell=0)} = \frac{LP}{r^3}, \tag{4.32}$$

and we also have three $\ell = 2$ modes

$$ {}^{(1)}KH_2{}^{(\ell=2)} = -\frac{4LP}{r^3}, \tag{4.33}$$

$$ {}^{(1)}KK^{(\ell=2)} = \frac{5LP}{r^3}, \tag{4.34}$$

$$ {}^{(1)}KG^{(\ell=2)} = \frac{LP}{r^3}. \tag{4.35}$$

Note that our findings at first order agree with [25], except for a relative minus sign for all the extrinsic curvature perturbations. At second order, however, our calculations yield different results again. For the $\ell = 0$ modes we find

$$ {}^{(2)}Kh_1{}^{(\ell=0)} = -\frac{13L^3P}{8r\sqrt{r(r-2M)}\left(\sqrt{r-2M}+\sqrt{r}\right)^4}, \tag{4.36}$$

$$ {}^{(2)}KK^{(\ell=0)} = \frac{L^3P\left(M^2 - 4Mr + 2M\sqrt{r(r-2M)} - 2\sqrt{r^3(r-2M)} + 2r^2\right)}{M^4r^3}, \tag{4.37}$$

and for the $\ell = 2$ modes we obtain

$$^{(2)}KH_2{}^{(\ell=2)} = -\frac{96L^3P}{7r^3\left(\sqrt{r-2M}+\sqrt{r}\right)^4}, \tag{4.38}$$

$$^{(2)}Kh_1{}^{(\ell=2)} = \frac{32L^3P}{7r\sqrt{r(r-2M)}\left(\sqrt{r-2M}+\sqrt{r}\right)^4}, \tag{4.39}$$

$$^{(2)}KK^{(\ell=2)} = -\frac{4L^3P\left(M^2-4Mr+2M\sqrt{r(r-2M)}-2\sqrt{r^3(r-2M)}+2r^2\right)}{7M^4r^3}, \tag{4.40}$$

$$^{(2)}KG^{(\ell=2)} = \frac{3L^3P\left(M^2-4Mr+2M\sqrt{r(r-2M)}-2\sqrt{r^3(r-2M)}+2r^2\right)}{7M^4r^3}. \tag{4.41}$$

4.3 Gauge Transformations

Now we will take advantage of the remaining freedom to fix our system in a gauge that makes the rest of our calculations as convenient as possible. Note that the form of the gauge transformation in Eq. (2.22) given by [45], which we will use here, differs from the conventions used in [25]. There, they used Eq. (22) from [16]. This follows from a different convention for the infinitesimal transformation (see App. A). Both conventions are equivalent, since it essentially comes down to a different choice of $^{(2)}\xi^\mu$ (see Sec. III from [46]). We opt for the conventions from [45] as it has a clear geometrical interpretation in terms of generators for Lie dragging (see App. A). At second order, the different conventions will yield different results, so from this point on it will not be fruitful to compare second order expressions.

4.3.1 First order gauge transformation

As discussed, we take a step by step approach and first fix the first order perturbations as desired. This transformation is generated by $^{(1)}\xi^\mu$ and will change the perturbations as

$$\begin{aligned} ^{(1)}g'_{\mu\nu} &= {}^{(1)}g_{\mu\nu} + \mathcal{L}_{^{(1)}\xi}\, {}^{(0)}g_{\mu\nu}, \\ ^{(2)}g'_{\mu\nu} &= {}^{(2)}g_{\mu\nu} + \mathcal{L}_{^{(1)}\xi}\, {}^{(1)}g_{\mu\nu} + \frac{1}{2}\mathcal{L}^2_{^{(1)}\xi}\, {}^{(0)}g_{\mu\nu}. \end{aligned}$$

We want to gauge fix the perturbations in a way that make our calculations as convenient as possible. As has already been discussed briefly in the introduction, one obtains a source term at second order that is quadratic in the first order perturbations. Therefore, we would like to remove all $\ell = 0$ modes so that the source term for the second order $\ell = 2$ wavefunction only has quadratic $\ell = 2$ contributions and no cross terms of monopoles and quadrupoles. Recall that there are no $\ell = 0$ contributions in the metric at first order, but there are first order $\ell = 0$ contributions for the extrinsic curvature. Hence, at first order, the gauge transformation amounts to removing the monopoles of the extrinsic curvature, given in Eqs. (4.31) and (4.32).

This first order gauge transformation will alter the second order perturbations as well. We lose the important feature that $H_0 = H_1 = h_1 = 0$ up to second order. These quantities being zero essentially means that the perturbative lapse and shit are zero, which allows for an easy identification between initial time derivatives of metric perturbations and the extrinsic curvature. This greatly simplifies the formulation of initial conditions for the Zerilli equation, which we want to solve numerically. The second order transformation therefore restores $H_0 = H_1 = h_0 = 0$ up to second order.

First, we implement the first order gauge transformation by choosing a ${}^{(1)}\xi^{\mu}$, such that the $\ell = 0$ modes of the extrinsic curvature at first order vanish. To determine the generator ${}^{(1)}\xi^{\mu}$, we decompose it in multipoles as

$$ {}^{(1)}\xi_a = \sum_{\ell} {}^{(1)}\mathcal{A}_a^{(\ell)}(r,t)\, P_\ell(\cos(\theta)), \quad {}^{(1)}\xi_\theta = \sum_{\ell} {}^{(1)}\mathcal{B}^{(\ell)}(r,t)\, \partial_\theta P_\ell(\cos(\theta)), \quad {}^{(1)}\xi_\varphi = 0. \tag{4.42} $$

The decomposition of gauge transfomations into spherical harmonics is covered extensively in Appendix C.1. From Eq. (C.16) and Eq. (C.22), it follows that we should have

$$ 2\mathcal{D}_{(a}\,{}^{(1)}\mathcal{A}_{b)}^{(\ell=0)} = -2t\sqrt{1-\frac{2M}{r}}\,{}^{(1)}Kf_{ab}^{(\ell=0)}, $$
$$ \frac{2}{r}\left(1-\frac{2M}{r}\right){}^{(1)}\mathcal{A}_r^{(\ell=0)} = -2t\sqrt{1-\frac{2M}{r}}\,{}^{(1)}KK^{(\ell=0)}, $$

where Kf_{ab} is defined similarly to f_{ab} in Eq. (C.14), but with metric perturbations replaced by extrinsic curvature perturbations. After working out the equations for each component of ${}^{(1)}Kf_{ab}^{(\ell=0)}$, we find the following set of four equations that determines the components of our first order generator

$$ 2\partial_t\,{}^{(1)}\mathcal{A}_t^{(\ell=0)} - \frac{2M}{r^2}\left(1-\frac{2M}{r}\right){}^{(1)}\mathcal{A}_r^{(\ell=0)} = 0, \tag{4.43} $$

$$ \partial_t\,{}^{(1)}\mathcal{A}_r^{(\ell=0)} + \partial_r\,{}^{(1)}\mathcal{A}_t^{(\ell=0)} - \frac{2M}{r^2}\frac{1}{1-2M/r}\,{}^{(1)}\mathcal{A}_t^{(\ell=0)} = 0, \tag{4.44} $$

$$ 2\partial_r\,{}^{(1)}\mathcal{A}_r^{(\ell=0)} + \frac{2M}{r^2}\frac{1}{1-2M/r}\,{}^{(1)}\mathcal{A}_r^{(\ell=0)} = -\frac{4LPt}{r^{5/2}\sqrt{r-2M}}, \tag{4.45} $$

$$ \frac{2}{r}\left(1-\frac{2M}{r}\right){}^{(1)}\mathcal{A}_r^{(\ell=0)} = \frac{2LPt\sqrt{r-2M}}{r^{7/2}}. \tag{4.46} $$

It follows trivially from Eq. (4.46) that

$$ {}^{(1)}\mathcal{A}_r^{(\ell=0)} = \frac{LPt}{r^{3/2}\sqrt{r-2M}}. \tag{4.47} $$

Note this is also a solution to Eq. (4.45). To solve for ${}^{(1)}\mathcal{A}_t^{(\ell=0)}$, we substitute the solution Eq. (4.47) into Eq.(4.44) to find the equation

$$ \partial_r\,{}^{(1)}\mathcal{A}_t^{(\ell=0)} - \frac{2M}{r^2}\frac{1}{1-\frac{2M}{r}}\,{}^{(1)}\mathcal{A}_t^{(\ell=0)} = -\frac{LP}{r^{3/2}\sqrt{r-2M}}, $$

which is solved by

$$ {}^{(1)}\mathcal{A}_t^{(\ell=0)} = \frac{LP\sqrt{r-2M}}{M\sqrt{r}}. \tag{4.48} $$

Unfortunately, this is not a solution to Eq. (4.43), so it is not possible to set all $\ell = 0$ components to zero with this simple ansatz. As a consequence, we are left with one remaining first order $\ell = 0$ perturbation in the ${}^{(1)}g_{tt}$ component. As a result of this non-vanishing component, there will be a non-vanishing first order (and consequently second order) lapse function. In this case, Eq. (2.20) is not valid anymore for the $\ell = 0$ modes. This is of no big influence as all other $\ell = 0$ perturbations vanish at first order, so the initial data (γ_{ab}, K_{ab}) is still free of first order $\ell = 0$ perturbations. At second order, where the non-vanishing perturbative lapse could still pose a problem, we can still use the gauge freedom to remove the non-vanishing lapse for the $\ell = 0$ modes. The major problem is that this component will give rise to some $\ell = 0$ cross terms with $\ell = 2$ quadrupoles in the source term.[4]

Raising the indices of the generator ${}^{(1)}\xi_\mu$ with the background metric ${}^{(0)}g^{\mu\nu}$, the vector ${}^{(1)}\xi^\mu$ for the first order transformation is given by

$$ {}^{(1)}\xi^t = -\frac{LP\sqrt{r}}{M\sqrt{r-2M}}, \quad {}^{(1)}\xi^r = \frac{LPt\sqrt{r-2M}}{r^{5/2}}, \quad {}^{(1)}\xi^A = 0. \tag{4.49} $$

Note this is the same generator as was used in [25]. Since we still need the spacetime metric $g_{\mu\nu}$, instead of the spatial metric γ_{ab}, we will refrain projecting onto the initial slice just yet and give the perturbations of $g_{\mu\nu}$ which will include t-dependencies. After the first order transformation, we have one $\ell = 0$ piece, as explained before, given by

$$ {}^{(1)}{H'_0}^{(\ell=0)} = -\frac{2LMPt}{r^{7/2}\sqrt{r-2M}}. \tag{4.50} $$

For the $\ell = 2$ modes at first order, we have the following non-vanishing perturbations

$$ \begin{aligned} {}^{(1)}{H'_2}^{(\ell=2)} &= \frac{16L^2M}{\sqrt{r}\left(\sqrt{r-2M}+\sqrt{r}\right)^5} + 8LPt\sqrt{\frac{r-2M}{r^7}}, \\ {}^{(1)}{K'}^{(\ell=2)} &= \frac{16L^2M}{\sqrt{r}\left(\sqrt{r-2M}+\sqrt{r}\right)^5} - 10LPt\sqrt{\frac{r-2M}{r^7}}, \\ {}^{(1)}{G'}^{(\ell=2)} &= -2LPt\sqrt{\frac{r-2M}{r^7}}. \end{aligned} $$

Note that these components follow directly from Eq. (2.21) and were not altered by the gauge transformation, since it only affects $\ell = 0$ monopoles. We are not able to compare these quantities to [25] at this point, since the first order quantities after the first order transformation are not stated explicitly.

As a consequence of the first order transformation, the second order perturbations are also altered. Since some of the expressions get rather lengthy, we will abbreviate the r-dependence of some of the perturbations. For the full expressions, we refer to the `HeadOnCollision.nb` Mathematica notebook [43]:

$$ \begin{aligned} {}^{(2)}{H'_0}^{(\ell=0)} =& \frac{L^2MP^2t^2(9M-4r)}{r^7(2M-r)} - \frac{L^2P^2}{r^3(2M-r)}, \\ {}^{(2)}{H'_1}^{(\ell=0)} =& \frac{L^2P^2t(3M-2r)}{r^5(r-2M)}, \\ {}^{(2)}{H'_2}^{(\ell=0)} =& L^4A'_1(r) + L^2P^2\left[A'_2(r) + q_0A'_3(r) + A'_4(r)t^2\right], \\ {}^{(2)}{K'}^{(\ell=0)} =& L^4B'_1(r) + L^2P^2\left[B'_2(r) + q_0B'_3(r) + B'_4(r)t^2\right] + L^3PB'_5(r)t, \end{aligned} $$

where the factors $A'_1(r), A'_2(r)\ldots$ and $B'_1(r), B'_2(r)\ldots$ are abbreviations for long factors which depend on r and M. It turns out that $A'_1(r) = B'_1(r)$ and $A'_3(r) = B'_3(r)$. For the $\ell = 2$ modes at second order, we have

[4] As we will see in Sec. 4.4, these cross terms turn out to not contribute, since the first order $\ell = 0$ perturbations of the initial data, and as a consequence ${}^{(1)}\psi^{(\ell=0)}$, vanish.

found that

$$\begin{aligned}
{}^{(2)}H_1'^{(\ell=2)} =& \frac{16L^3MP}{r^2\sqrt{r-2M}\left(\sqrt{r-2M}+\sqrt{r}\right)^5},\\
{}^{(2)}H_2'^{(\ell=2)} =& L^4C_1'(r)+L^2P^2\left(C_2'(r)+q_2C_3'(r)\right)+L^3PC_4'(r)t,\\
{}^{(2)}h_1'^{(\ell=2)} =& -\frac{64L^3Pt}{7r^2\left(\sqrt{r-2M}+\sqrt{r}\right)^4},\\
{}^{(2)}K'^{(\ell=2)} =& L^4D_1'(r)+L^2P^2\left(D_2'(r)+q_2D_3'(r)\right)+L^3PD_4'(r)t,\\
{}^{(2)}G'^{(\ell=2)} =& -\frac{6L^3Pt\sqrt{r-2M}\left(M^2-2\sqrt{r^3(r-2M)}-4Mr+2M\sqrt{r(r-2M)}+2r^2\right)}{7M^4r^{7/2}}.
\end{aligned}$$

Again $C_1'(r), C_2'(r), \ldots$ and $D_1'(r), D_2'(r), \ldots$ are abbreviations for long terms. In this case, we have that $C_1'(r) = D_1'(r)$, $C_2'(r) = D_2'(r)$ and $C_3'(r) = D_3'(r)$.

4.3.2 Second order gauge transformation

At second order, we still have the freedom to make a choice of coordinates and fix the gauge. This second order transformation, generated by ${}^{(2)}\xi^\mu$, changes the metric as follows

$$\begin{aligned}
{}^{(1)}g''_{\mu\nu} &= {}^{(1)}g'_{\mu\nu},\\
{}^{(2)}g''_{\mu\nu} &= {}^{(2)}g'_{\mu\nu} + \mathcal{L}_{{}^{(2)}\xi}\,{}^{(0)}g_{\mu\nu}.
\end{aligned}$$

Before the first order transformation, we had the nice property that the perturbative lapse and shift all vanished. This allowed us to easily relate the extrinsic curvature to time derivatives of the metric perturbations, via Eq. (2.20). At second order, we would like to restore the condition $H_0 = H_1 = h_1 = 0$ to make the identification between the extrinsic curvature and time derivatives of the metric as easy as possible.[5]

To find a suitable generator ${}^{(2)}\xi^\mu$, we again decompose this vector in terms of its multipoles and solve the corresponding equations for each ℓ separately. The equations take the same form as Eqs. (C.16)–(C.22), but now the first order coefficients are replaced by second order ones. For $\ell = 0$, this yields the following set of equations

$$\begin{aligned}
2\partial_t\,{}^{(2)}\mathcal{A}_t^{(\ell=0)} - \frac{2M}{r^2}\left(1-\frac{2M}{r}\right){}^{(2)}\mathcal{A}_r^{(\ell=0)} &= -\frac{L^2P^2}{r^4} + \frac{L^2MP^2(9M-4r)}{r^8}t^2,\\
\partial_t\,{}^{(2)}\mathcal{A}_r^{(\ell=0)} + \partial_r\,{}^{(2)}\mathcal{A}_t^{(\ell=0)} - \frac{2M}{r^2}\frac{1}{1-\frac{2M}{r}}\,{}^{(2)}\mathcal{A}_t^{(\ell=0)} &= \frac{L^2P^2(3M-2r)}{r^5(2M-r)}t,\\
{}^{(2)}\mathcal{A}_t^{(\ell=0)} + \partial_t\,{}^{(2)}\mathcal{B}^{(\ell=0)} &= 0.
\end{aligned}$$

To solve this system of differential equations, we make the ansatz that all coefficients are polynomials in time, since we are looking for local solutions near the initial time slice Σ_0. This is the same ansatz we applied in

[5] Since at first order ${}^{(1)}H_0'^{(\ell=0)}$ does not vanish, it is not possible to use Eq. (2.20) for the $\ell = 0$ pieces, whatever the second order gauge might be.

the first order case. Specifically, we make the ansatz

$$
\begin{aligned}
{}^{(2)}\mathcal{A}_t^{(\ell=0)}(t,r) &= \sum_{n=0}^{\infty} t^n A_t^{(n)}(r), \\
{}^{(2)}\mathcal{A}_r^{(\ell=0)}(t,r) &= \sum_{n=0}^{\infty} t^n A_r^{(n)}(r), \\
{}^{(2)}\mathcal{B}^{(\ell=0)}(t,r) &= \sum_{n=0}^{\infty} t^n B^{(n)}(r),
\end{aligned}
$$

where we dropped the $(\ell = 0)$ superscript in the t-expansion for notational convenience. This ansatz creates an infinite ladder of equations in t^n. The system permits it first solution when we carry out the expansion up and till t^2. Hence, we neglect all $\mathcal{O}(t^3)$ terms and find the following simplified system of equations

$$
\frac{2M}{r^2}\left(1-\frac{2M}{r}\right)A_r^{(2)} = \frac{L^2 M P^2 (9M-4r)}{r^8}, \tag{4.51}
$$

$$
2A_r^{(2)} + \partial_r A_t^{(1)} - \frac{2M}{r^2}\left(1-\frac{2M}{r}\right)^{-1} A_t^{(1)} = \frac{L^2 P^2 (3M-2r)}{r^5(2M-r)}, \tag{4.52}
$$

$$
2A_t^{(1)} - \frac{2M}{r^2}\left(1-\frac{2M}{r}\right)A_r^{(0)} = -\frac{L^2 P^2}{r^4}, \tag{4.53}
$$

$$
2A_t^{(1)} + B^{(2)} = 0, \tag{4.54}
$$

which can easily be solved equation by equation. First, we rearrange the factor in Eq. (4.51) to find

$$
A_r^{(2)}(r) = \frac{L^2 P^2 (9M-4r)}{2r^5(2M-r)}.
$$

Then, we substitute this expression into Eq. (4.52) and solve the resulting linear ordinary differential equation for $A_t^{(1)}(r)$ to find

$$
A_t^{(1)}(r) = \frac{L^2 P^2 \left(2M\left(4M^3 + 2M^2 r + 3Mr^2 - 3r^3\right) + 3r^3(r-2M)\ln\left(\frac{r}{r-2M}\right)\right)}{8M^4 r^4}.
$$

The solution for $B^{(2)}(r)$ follows trivially from Eq. (4.54), at this point. Finally, we can plug this solution back into Eq. (4.53) which yields

$$
A_r^{(0)}(r) = -\frac{L^2 P^2 \left(\frac{2M\left(6M^3+2M^2 r+3Mr^2-3r^3\right)}{2M-r} - 3r^3 \ln\left(\frac{r}{r-2M}\right)\right)}{8M^5 r}.
$$

Hence, we have found that for the $\ell = 0$ modes the generator ${}^{(2)}\xi_\mu^{(\ell=0)}$ has components

$$
{}^{(2)}\mathcal{A}_t^{(\ell=0)}(t,r) = A_t^{(1)}(r)t, \quad {}^{(2)}\mathcal{A}_r^{(\ell=0)}(t,r) = A_r^{(0)}(r) + A_r^{(2)}(r)t^2, \quad {}^{(2)}\mathcal{B}^{(\ell=0)}(t,r) = B^{(2)}(r)t^2.
$$

The $\ell = 2$ components can be determined in a similar fashion. In this case, we have the system of equations

$$
\begin{aligned}
2\partial_t {}^{(2)}\mathcal{A}_t^{(\ell=2)} - \frac{2M}{r^2}\left(1-\frac{2M}{r}\right){}^{(2)}\mathcal{A}_r^{(\ell=0)} = 0,\\
\partial_t {}^{(2)}\mathcal{A}_r^{(\ell=2)} + \partial_r {}^{(2)}\mathcal{A}_t^{(\ell=2)} - \frac{2M}{r^2}\frac{1}{1-\frac{2M}{r}}{}^{(2)}\mathcal{A}_t^{(\ell=2)} = -\frac{16L^3MP}{r^2\sqrt{r-2M}\left(\sqrt{r-2M}+\sqrt{r}\right)^5},\\
{}^{(2)}\mathcal{A}_t^{(\ell=0)} + \partial_t {}^{(2)}\mathcal{B}^{(\ell=0)} = 0.
\end{aligned}
$$

By applying the same ansatz as before, we ultimately find that ${}^{(2)}\xi_\mu^{(\ell=2)}$ has to have the components

$$
\begin{aligned}
{}^{(2)}\mathcal{A}_t^{(\ell=2)}(t,r) =& -\frac{2L^3P\left(4\sqrt{r^3(r-2M)}+8Mr-4r^2-9M\sqrt{r(r-2M)}\right)}{M^4r}\\
&+\frac{5L^3P(r-2M)\ln\left(\frac{r}{r-2M}\right)}{M^3r}+\frac{4(r-2M)\ln\left(\frac{1}{\sqrt{\frac{r}{r-2M}}}+1\right)}{M^3r},\\
{}^{(2)}\mathcal{A}_r^{(\ell=2)}(t,r) =& 0,\\
{}^{(2)}\mathcal{B}^{(\ell=2)}(t,r) =& -{}^{(2)}\mathcal{A}_t^{(\ell=2)}(t,r).
\end{aligned}
$$

Now the overall generator ${}^{(2)}\xi_\mu$ is simply given by

$$
\begin{aligned}
{}^{(2)}\xi_t &= {}^{(2)}\mathcal{A}_t^{(\ell=0)}(t,r) + {}^{(2)}\mathcal{A}_t^{(\ell=2)}(t,r)P_2(\cos\theta),\\
{}^{(2)}\xi_r &= {}^{(2)}\mathcal{A}_r^{(\ell=0)}(t,r),\\
{}^{(2)}\xi_A &= {}^{(2)}\mathcal{B}^{(\ell=2)}(t,r)D_AP_2(\cos\theta).
\end{aligned}
$$

Thereby achieving that ${}^{(2)}H_0'' = {}^{(2)}H_1'' = {}^{(2)}h_1'' = 0$ up to $\mathcal{O}(t^2)$.

4.3.3 Projecting onto the initial time slice

Now that we have gauge fixed our original 4d-metric $g_{\mu\nu}$ from Eq. (2.21) up to second order to $g''_{\mu\nu}$, we would like to recover the spatial metric $\gamma''_{\mu\nu}$ and extrinsic curvature $K''_{\mu\nu}$ on the $t = 0$ slice. The initial data can be recovered from $g''_{\mu\nu}$ by first calculating the normal vector n''_μ to determine $(\gamma''_{\mu\nu}, K''_{\mu\nu})$ and then taking the limit $t \to 0$. First observe that the spatial metric $\gamma''_{\mu\nu}$ is related to the $g''_{\mu\nu}$ via

$$
\gamma''_{\mu\nu} = g''_{\mu\nu} + n''_\mu n''_\nu. \tag{4.55}
$$

Recall that after the gauge transformations the perturbative lapse does no longer vanish, so we have to determine the perturbative expansion of n''_μ. To this end, we expand the lapse function and shift vector as

$$
N'' = {}^{(0)}N'' + \epsilon\,{}^{(1)}N'' + \epsilon^2\,{}^{(2)}N'' + \mathcal{O}(\epsilon^3), \qquad N''^a = {}^{(0)}N''^a + \epsilon\,{}^{(1)}N''^a + \epsilon^2\,{}^{(2)}N''^a + \mathcal{O}(\epsilon^3),
$$

and substitute this into Eq. (2.18), so that the metric $g''_{\mu\nu}$ can be expanded in ϵ as

$$\begin{aligned} g''_{\mu\nu}dx^\mu dx^\nu = &- {}^{(0)}N''^2 dt^2 + {}^{(0)}\gamma''_{ab}(dx^a + {}^{(0)}N''^a dt)(dx^b + {}^{(0)}N''^b dt) \\ &+ \epsilon\Big[-2\,{}^{(0)}N''\,{}^{(1)}N'' dt^2 + {}^{(1)}\gamma''_{ab}(dx^a + {}^{(0)}N''^a dt)(dx^b + {}^{(0)}N''^b dt) \\ &+ 2\,{}^{(0)}\gamma''_{ab}\,{}^{(1)}N''^a dt dx^a\Big] \\ &+ \epsilon^2\Big[-\Big({}^{(1)}N''^2 + 2\,{}^{(0)}N''\,{}^{(2)}N''\Big) dt^2 + {}^{(2)}\gamma''_{ab}(dx^a + {}^{(0)}N''^a dt)(dx^b + {}^{(0)}N''^b dt) \\ &+ 2\,{}^{(1)}\gamma''_{ab}\,{}^{(1)}N''^a dt dx^a + {}^{(0)}\gamma''_{ab}\,{}^{(1)}N''^a\,{}^{(1)}N''^b dt^2 \\ &+ 2\,{}^{(0)}\gamma''_{ab}\,{}^{(2)}N''^a dt dx^a\Big] + \mathcal{O}(\epsilon^3). \end{aligned}$$

Since ${}^{(0)}N''^a = {}^{(0)}N^a = 0$ and ${}^{(0)}N'' = {}^{(0)}N = \sqrt{1-2M/r}$, as we have seen before, it follows that at first order the ADM quantities are given by

$$ {}^{(1)}N'' = -\frac{1}{2\,{}^{(0)}N''}\,{}^{(1)}g''_{00} = \frac{LMPt}{r^4}, \tag{4.56}$$

$$ {}^{(1)}N''^a = {}^{(0)}\gamma''^{ab}\,{}^{(1)}g''_{0b} = 0, \tag{4.57}$$

$$ {}^{(1)}\gamma''_{ab} = {}^{(1)}g''_{ab}, \tag{4.58}$$

where ${}^{(0)}\gamma''^{ab} = {}^{(0)}\gamma^{ab}$ is simply the spatial part of the Schwarzschild metric ${}^{(0)}g^{\mu\nu}$ and where we used that in our case ${}^{(0)}g''_{0b} = 0$. At second order, the relevant quantities are given by

$$\begin{aligned} {}^{(2)}N'' &= -\frac{1}{2\,{}^{(0)}N''}({}^{(2)}g''_{00} + {}^{(1)}N''^2) = -\frac{L^2P^2\left(-8M^2t^2 + 4Mrt^2 + r^4\right)}{2\sqrt{r^{15}(r-2M)}}, \\ {}^{(2)}N''^a &= {}^{(0)}\gamma''^{ab}\,{}^{(2)}g''_{0b} = 0, \\ {}^{(2)}\gamma''_{ab} &= {}^{(2)}g''_{ab}, \end{aligned}$$

since ${}^{(2)}g''_{0b} = 0$ for our choice of gauge. Now, the normal covector n''_μ can be expanded as

$$ {}^{(i)}n''_\mu = \left(-{}^{(i)}N'', 0, 0, 0\right).$$

Using the perturbative covector, Eq. (4.55) can be arranged order by order as

$$\begin{aligned} {}^{(0)}\gamma''_{\mu\nu} &= {}^{(0)}g''_{\mu\nu} + {}^{(0)}n''_\mu\,{}^{(0)}n''_\nu, \\ {}^{(1)}\gamma''_{\mu\nu} &= {}^{(1)}g''_{\mu\nu} + {}^{(1)}n''_\mu\,{}^{(0)}n''_\nu + {}^{(0)}n''_\mu\,{}^{(1)}n''_\nu, \\ {}^{(2)}\gamma''_{\mu\nu} &= {}^{(2)}g''_{\mu\nu} + {}^{(1)}n''_\mu\,{}^{(1)}n''_\nu + {}^{(2)}n''_\mu\,{}^{(0)}n''_\nu + {}^{(0)}n''_\mu\,{}^{(2)}n''_\nu. \end{aligned}$$

Secondly, we want to recover the extrinsic curvature. Note that $K''_{\mu\nu} = \frac{1}{2}\mathcal{L}_{n''}\gamma''_{\mu\nu}$. This will involve the normal vector n''^μ. Therefore, we need to raise the index of the covector n''_μ. Since we are working in second order perturbation theory, we have to take particular care in working out $n''^\mu = g''^{\mu\nu}n''_\nu$, where we have to contract over the full metric and not just the background metric. In general, the inverse metric $g^{\mu\nu}$ of some arbitrary metric can be expanded order by order as

$$\begin{aligned} g^{\mu\nu} = & \ {}^{(0)}g^{\mu\nu} \\ & - \epsilon \ {}^{(0)}g^{\mu\alpha} \ {}^{(0)}g^{\nu\beta} \ {}^{(1)}g_{\alpha\beta} \\ & - \epsilon^2 \left[\ {}^{(0)}g^{\mu\alpha} \ {}^{(0)}g^{\nu\beta} \ {}^{(2)}g_{\alpha\beta} - \ {}^{(0)}g^{\mu\alpha} \ {}^{(0)}g^{\nu\beta} \ {}^{(0)}g^{\lambda\kappa} \ {}^{(1)}g_{\lambda\alpha} \ {}^{(1)}g_{\kappa\beta} \right] + \mathcal{O}(\epsilon^3), \end{aligned} \tag{4.59}$$

as deduced from Eq. (B.4). The index of some covector ω_μ can thus be raised in second order perturbation theory as

$$\begin{aligned} \omega^\mu = & g^{\mu\nu}\omega_\nu \\ = & \ {}^{(0)}g^{\mu\nu} \, {}^{(0)}\omega_\nu \\ & + \epsilon \left[\ {}^{(0)}g^{\mu\nu} \, {}^{(1)}\omega_\nu - \ {}^{(0)}g^{\mu\alpha} \ {}^{(0)}g^{\nu\beta} \ {}^{(1)}g_{\alpha\beta} \ {}^{(0)}\omega_\nu \right] \\ & + \epsilon^2 \Big[\ {}^{(0)}g^{\mu\nu} \, {}^{(2)}\omega_\nu - \ {}^{(0)}g^{\mu\alpha} \ {}^{(0)}g^{\nu\beta} \ {}^{(1)}g_{\alpha\beta} \ {}^{(1)}\omega_\nu \\ & - \left(\ {}^{(0)}g^{\mu\alpha} \ {}^{(0)}g^{\nu\beta} \ {}^{(2)}g_{\alpha\beta} - \ {}^{(0)}g^{\mu\alpha} \ {}^{(0)}g^{\nu\beta} \ {}^{(0)}g^{\lambda\kappa} \ {}^{(1)}g_{\lambda\alpha} \ {}^{(1)}g_{\kappa\beta} \right) {}^{(0)}\omega_\nu \Big] + \mathcal{O}(\epsilon^3). \end{aligned}$$

When we apply this to n''_μ we find the following first and second order normal vectors

$$ {}^{(1)}n''^\mu = \left(-\frac{LPMt}{r^3(r-2M)}, 0, 0, 0 \right), \quad {}^{(2)}n''^\mu = \left(\frac{3L^2P^2M^2t^2}{2r^{13/2}(r-2M)^{3/2}}, 0, 0, 0 \right). \tag{4.60}$$

The extrinsic curvature ${}^{(i)}K''_{ab}$ can now be calculated order by order from ${}^{(i)}n''^\mu$ and ${}^{(i)}\gamma''_{ab}$

$$\begin{aligned} K''_{ab} = & \frac{1}{2}\mathcal{L}_{n''}\gamma''_{ab} \\ = & \frac{1}{2}\left(n''^\lambda \partial_\lambda \gamma''_{ab} + \gamma''_{\lambda b}\partial_a n''^\lambda + \gamma''_{a\lambda}\partial_b n''^\lambda \right) \\ = & \frac{1}{2}\left({}^{(0)}n''^\lambda \partial_\lambda {}^{(0)}\gamma''_{ab} + {}^{(0)}\gamma''_{\lambda b}\partial_a {}^{(0)}n''^\lambda + {}^{(0)}\gamma''_{a\lambda}\partial_b {}^{(0)}n''^\lambda \right) \\ & + \frac{1}{2}\epsilon \Big({}^{(0)}n''^\lambda \partial_\lambda {}^{(1)}\gamma''_{ab} + {}^{(1)}\gamma''_{\lambda b}\partial_a {}^{(0)}n''^\lambda + {}^{(1)}\gamma''_{a\lambda}\partial_b {}^{(0)}n''^\lambda \\ & + {}^{(1)}n''^\lambda \partial_\lambda {}^{(0)}\gamma''_{ab} + {}^{(0)}\gamma''_{\lambda b}\partial_a {}^{(1)}n''^\lambda + {}^{(0)}\gamma''_{a\lambda}\partial_b {}^{(1)}n''^\lambda \Big) \\ & + \frac{1}{2}\epsilon^2 \Big({}^{(0)}n''^\lambda \partial_\lambda {}^{(2)}\gamma''_{ab} + {}^{(2)}\gamma''_{\lambda b}\partial_a {}^{(0)}n''^\lambda + {}^{(2)}\gamma''_{a\lambda}\partial_b {}^{(0)}n''^\lambda \\ & + {}^{(1)}n''^\lambda \partial_\lambda {}^{(1)}\gamma''_{ab} + {}^{(1)}\gamma''_{\lambda b}\partial_a {}^{(1)}n''^\lambda + {}^{(1)}\gamma''_{a\lambda}\partial_b {}^{(1)}n''^\lambda \\ & + {}^{(2)}n''^\lambda \partial_\lambda {}^{(0)}\gamma''_{ab} + {}^{(0)}\gamma''_{\lambda b}\partial_a {}^{(2)}n''^\lambda + {}^{(0)}\gamma''_{a\lambda}\partial_b {}^{(2)}n''^\lambda \Big) + \mathcal{O}(\epsilon^3). \end{aligned} \tag{4.61}$$

The only remaining step is to project the quantities $(\gamma''_{ab}, K''_{ab})$ on the initial surface Σ_0 by taking the limit $t \to 0$. At first order, the spatial metric's perturbations consist only of the $\ell = 2$ modes

$$ {}^{(1)}H_2''^{(\ell=2)} = {}^{(1)}K''^{(\ell=2)} = \frac{16L^2M}{\sqrt{r}\left(\sqrt{r-2M}+\sqrt{r}\right)^5}, \tag{4.62}$$

which agrees with [25]. Furthermore, at first order, the extrinsic curvature only has the following $\ell = 2$ modes

$$
{}^{(1)}KH_2''^{(\ell=2)} = -\frac{4LP}{r^3}, \tag{4.63}
$$

$$
{}^{(1)}KK''^{(\ell=2)} = \frac{5LP}{r^3}, \tag{4.64}
$$

$$
{}^{(1)}KG''^{(\ell=2)} = \frac{LP}{r^3}. \tag{4.65}
$$

Up to an overall minus sign for all three perturbations, these components agree with [25]. Thus, as desired, the first order perturbations of the initial data have no $\ell = 0$ contributions as instated by the first order gauge transformation. This is also evident from Eq. (4.61). Most terms feature the contraction of n''^{μ}, which only has a temporal components with γ''_{ab} which only has spatial components. The only contributing term is ${}^{(0)}n''^t \partial_t {}^{(2)}\gamma''_{ab}$, which recovers the familiar relation in Eq. (2.20).

At second order, we start seeing notable differences from [25] again. In our calculations we find the following set of $\ell = 0$ modes of ${}^{(2)}\gamma''_{ab}$

$$
{}^{(2)}H_2''^{(\ell=0)} = L^4 A_1''(r) + L^2 P^2 \left[A_2''(r) + q_0 A_3''(r)\right], \tag{4.66}
$$

$$
{}^{(2)}K''^{(\ell=0)} = L^4 B_1''(r) + L^2 P^2 \left[A_2''(r) + q_0 B_3''(r)\right], \tag{4.67}
$$

where we have abbreviated the long terms again. Recall $A_1''(r) = B_1''(r)$ and $A_3''(r) = B_3''(r)$. The $\ell = 2$ modes are

$$
{}^{(2)}H_2''^{(\ell=2)} = {}^{(2)}K''^{(\ell=2)} = L^4 C_1''(r) + L^2 P^2 \left[C_2''(r) + q_2 C_3''(r)\right]. \tag{4.68}
$$

The second order perturbations of the extrinsic curvature are given by the monopoles

$$
{}^{(2)}KK''^{(\ell=0)} = \frac{L^3 P \left(M^2 - 2\sqrt{r^3(r-2M)} - 4Mr + 2M\sqrt{r(r-2M)} + 2r^2\right)}{M^4 r^3}, \tag{4.69}
$$

and the quadrupoles

$$
{}^{(2)}KH_2''^{(\ell=2)} = -\frac{4L^3 P \left(126M^2 + 24\left(\sqrt{r^3(r-2M)} + r^2\right) + M\left(-83\sqrt{r(r-2M)} - 111r\right)\right)}{7r^{7/2}(r-2M)\left(\sqrt{r-2M} + \sqrt{r}\right)^5}, \tag{4.70}
$$

$$
{}^{(2)}Kh_1''^{(\ell=2)} = L^3 P D_1''(r), \tag{4.71}
$$

$$
{}^{(2)}KK''^{(\ell=2)} = \frac{8L^3 P \left(21M^2 - 4\left(\sqrt{r^3(r-2M)} + r^2\right) + M\left(11\sqrt{r(r-2M)} + 15r\right)\right)}{7r^{7/2}\sqrt{r-2M}\left(\sqrt{r-2M} + \sqrt{r}\right)^6}, \tag{4.72}
$$

$$
{}^{(2)}KG''^{(\ell=2)} = L^3 P E_1''(r). \tag{4.73}
$$

For the full form of the abbreviated terms, we again refer to `HeadOnCollission_final.nb` [43]. Apart from the L^4-term, which is the same everywhere, our perturbations take on a quite different form from [25]. A notable difference, for instance, is that in our case the perturbations of ${}^{(2)}\gamma''_{ab}$ we do not have a ${}^{(2)}G_2''^{(\ell=2)}$ contribution, like in the calculations of Nicasio *et al.*

4.4 Zerilli Equation

So far, we have analytically determined the initial data perturbations belonging to the BHs in a head-on collision. In order to make predictions about the physical behaviour of the system, such as gravitational wave signals, QNMs and horizon shapes, we need to evolve our initial data. Hence, we need to determine the master equation with which to evolve our perturbations.

For the even perturbations on a Schwarzschild background this is the Zerilli equation. We will first present the derivation of the Zerilli equation at first order in detail, since it serves as a template for the second order calculation. After the first order calculation, we proceed by repeating the same derivation at second order and taking the quadratic first order cross terms into account to obtain the second order Zerilli equation including its source term.

4.4.1 First Order

There are two approaches to deriving the Zerilli equation: Zerilli's original derivation that relies on the convenience of the Regge-Wheeler gauge [16, 22, 40] and Moncrief's alternative one which uses a variational approach and is gauge independent [41]. The advantage of Zerilli's approach is its simplicity, even at second order. On the other hand, Moncrief's master function is more convenient, because it is a gauge invariant combination of only the initial data. The derivation, however, is more involved, especially at second order. In this thesis, we opted for simplicity and we will follow Zerilli's approach. The calculations are worked out in the `M2xS2-Split_coordinates_Final.nb` Mathematica notebook [43].

In order to derive the Zerilli equation, we assume that the first-order perturbations satisfy the Regge-Wheeler gauge ${}^{(1)}G = {}^{(1)}h_0 = {}^{(1)}h_1 = 0$. The expressions for the Ricci tensor in this gauge can be found in Eq. (C.28)–(C.30). The Einstein equation $\delta R^{\mathrm{RW}}_{AB} = 0$, contains two independent pieces of information, each accompanied by a different harmonic. The first equality $-\frac{1}{2} f_c{}^c = 0$, belonging to $D_A D_B Y^{\ell m}$, implies that

$$ {}^{(1)}H_2{}^{\mathrm{RW}} = {}^{(1)}H_0{}^{\mathrm{RW}}, \tag{4.74} $$

and from the second equality, belonging to $\Omega_{AB} Y^{\ell m}$, we obtain a differential equation of second order in r

$$ \begin{aligned} \frac{\partial^2\, {}^{(1)}K^{\mathrm{RW}}}{\partial r^2} = {} & \frac{2}{r(r-2M)}\, {}^{(1)}H_0{}^{\mathrm{RW}} + \frac{2}{r} \frac{\partial {}^{(1)}H_0{}^{\mathrm{RW}}}{\partial r} - \frac{2}{r-2M} \frac{\partial {}^{(1)}H_1{}^{\mathrm{RW}}}{\partial t} \\ & + \frac{(\ell+2)(\ell-1)}{r(r-2M)}\, {}^{(1)}K^{\mathrm{RW}} - \frac{4r-6M}{r(r-2M)} \frac{\partial {}^{(1)}K^{\mathrm{RW}}}{\partial r} + \frac{r^2}{(r-2M)^2} \frac{\partial^2\, {}^{(1)}K^{\mathrm{RW}}}{\partial t^2}. \end{aligned} \tag{4.75} $$

The equations $\delta R^{\mathrm{RW}}_{tB} = 0$ and $\delta R^{\mathrm{RW}}_{rB} = 0$, respectively, yield the following two differential equations which are first order in r

$$ \frac{\partial {}^{(1)}H_1{}^{\mathrm{RW}}}{\partial r} = \frac{r}{r-2M} \frac{\partial {}^{(1)}H_0{}^{\mathrm{RW}}}{\partial t} + \frac{r}{r-2M} \frac{\partial {}^{(1)}K^{\mathrm{RW}}}{\partial t} - \frac{2M}{r\,(r-2M)}\, {}^{(1)}H_1{}^{\mathrm{RW}}, \tag{4.76} $$

$$ \frac{\partial {}^{(1)}H_0{}^{\mathrm{RW}}}{\partial r} = \frac{\partial {}^{(1)}K^{\mathrm{RW}}}{\partial r} - \frac{2M}{r\,(r-2M)}\, {}^{(1)}H_0{}^{\mathrm{RW}} + \frac{r}{r-2M} \frac{\partial {}^{(1)}H_1{}^{\mathrm{RW}}}{\partial t}, \tag{4.77} $$

and $\delta R^{\mathrm{RW}}_{rt} = 0$ yields the third differential equation of first order in r

$$ \frac{\partial^2\, {}^{(1)}K^{\mathrm{RW}}}{\partial t \partial r} = \frac{1}{r} \frac{\partial {}^{(1)}H_0{}^{\mathrm{RW}}}{\partial t} + \frac{\ell(\ell+1)}{2r^2}\, {}^{(1)}H_1{}^{\mathrm{RW}} - \frac{r-3M}{r\,(r-2M)} \frac{\partial {}^{(1)}K^{\mathrm{RW}}}{\partial t}. \tag{4.78} $$

By differentiating Eq. (4.77) with respect to t and, then, substituting Eq. (4.78) into it, the t and r derivative of ${}^{(1)}K^{\text{RW}}$ can be eliminated from Eq. (4.77) and we obtain

$$\frac{\partial^2\, {}^{(1)}H_0{}^{\text{RW}}}{\partial t \partial r} = \frac{r}{r-2M}\frac{\partial^2\, {}^{(1)}H_1{}^{\text{RW}}}{\partial t^2} + \frac{r-4M}{r\,(r-2M)}\frac{\partial\, {}^{(1)}H_0{}^{\text{RW}}}{\partial t} - \frac{r-3M}{r\,(r-2M)}\frac{\partial\, {}^{(1)}K^{\text{RW}}}{\partial t} + \frac{\ell(\ell+1)}{2r^2}\, {}^{(1)}H_1{}^{\text{RW}}. \quad (4.79)$$

The remaining Einstein equations $\delta R^{\text{RW}}_{tt} = 0$ and $\delta R^{\text{RW}}_{rr} = 0$ yield two differential equations, which are second order in r. These are, respectively, given by

$$\begin{aligned}\frac{1}{2}\frac{\partial^2\, {}^{(1)}H_0{}^{\text{RW}}}{\partial r^2} =& -\frac{1}{r-2M}\frac{\partial\, {}^{(1)}H_0{}^{\text{RW}}}{\partial r} - \frac{r^2}{2(r-2M)^2}\frac{\partial^2\, {}^{(1)}H_0{}^{\text{RW}}}{\partial t^2} \\ &+ \frac{\ell(\ell+1)}{2r^2}\frac{r}{r-2M}\, {}^{(1)}H_0{}^{\text{RW}} + \frac{2r-3M}{(r-2M)^2}\frac{\partial\, {}^{(1)}H_1{}^{\text{RW}}}{\partial t} \\ &+ \frac{r}{r-2M}\frac{\partial^2\, {}^{(1)}H_1{}^{\text{RW}}}{\partial t \partial r} + \frac{M}{r(r-2M)}\frac{\partial\, {}^{(1)}K^{\text{RW}}}{\partial r} \\ &- \frac{r^2}{(r-2M)^2}\frac{\partial^2\, {}^{(1)}K^{\text{RW}}}{\partial t^2},\end{aligned} \quad (4.80)$$

$$\begin{aligned}\frac{\partial^2\, {}^{(1)}K^{\text{RW}}}{\partial r^2} - \frac{1}{2}\frac{\partial^2\, {}^{(1)}H_0{}^{\text{RW}}}{\partial r^2} =& \frac{1}{r-2M}\frac{\partial\, {}^{(1)}H_0{}^{\text{RW}}}{\partial r} + \frac{r^2}{2(r-2M)^2}\frac{\partial^2\, {}^{(1)}H_0{}^{\text{RW}}}{\partial t^2} \\ &+ \frac{\ell(\ell+1)}{2r^2}\frac{r}{r-2M}\, {}^{(1)}H_0{}^{\text{RW}} - \frac{M}{(r-2M)^2}\frac{\partial\, {}^{(1)}H_1{}^{\text{RW}}}{\partial t} \\ &- \frac{r}{r-2M}\frac{\partial^2\, {}^{(1)}H_1{}^{\text{RW}}}{\partial t \partial r} + \frac{3M-2r}{r(r-2M)}\frac{\partial\, {}^{(1)}K^{\text{RW}}}{\partial r}.\end{aligned} \quad (4.81)$$

To isolate $\partial_r^2\, {}^{(1)}K^{\text{RW}}$, Eq. (4.80) and Eq. (4.81) can be added to each other. This yields

$$\frac{\partial^2\, {}^{(1)}K^{\text{RW}}}{\partial r^2} = \frac{\ell(\ell+1)}{r^2}\frac{r}{r-2M}\, {}^{(1)}H_0{}^{\text{RW}} + \frac{2}{r-2M}\frac{\partial\, {}^{(1)}H_1{}^{\text{RW}}}{\partial t} - \frac{2}{r}\frac{\partial\, {}^{(1)}K^{\text{RW}}}{\partial r} - \frac{r^2}{(r-2M)^2}\frac{\partial^2\, {}^{(1)}K^{\text{RW}}}{\partial t^2}. \quad (4.82)$$

By equating Eq. (4.82) to Eq. (4.75), we can eliminate the second order derivatives in r, to obtain the expression

$$\begin{aligned}&\frac{(\ell+2)(\ell-1)}{r(r-2M)}\, {}^{(1)}H_0{}^{\text{RW}} - \frac{2}{r}\frac{\partial\, {}^{(1)}H_0{}^{\text{RW}}}{\partial r} + \frac{4}{r-2M}\frac{\partial\, {}^{(1)}H_1{}^{\text{RW}}}{\partial t} + \frac{(\ell+2)(\ell-1)}{r(r-2M)}\, {}^{(1)}K^{\text{RW}} \\ &+ \frac{2r-2M}{r(r-2M)}\frac{\partial\, {}^{(1)}K^{\text{RW}}}{\partial r} - \frac{2r^2}{(r-2M)^2}\frac{\partial^2\, {}^{(1)}K^{\text{RW}}}{\partial t^2} = 0.\end{aligned}$$

Now we take the t derivative of this, which allows us to eliminate the remaining r derivatives by substituting Eqs. (4.78) and (4.79) in our expression. This way, we obtain a single non-trivial piece of information from the set of second order equations called the "algebraic identity"[6] [39, 40]

$$\begin{aligned}&-\frac{\ell(\ell+1)M}{r^2}\, {}^{(1)}H_1{}^{\text{RW}} - 2r\frac{\partial^2\, {}^{(1)}H_1{}^{\text{RW}}}{\partial t^2} - \left[(\ell-1)(\ell+1) + \frac{6M}{r^2}\right]\frac{\partial\, {}^{(1)}H_0{}^{\text{RW}}}{\partial t} \\ &+ \left[(\ell+2)(\ell-1) + \frac{2M(r-3M)}{r(r-2M)}\right]\frac{\partial\, {}^{(1)}K^{\text{RW}}}{\partial t} + \frac{2r^3}{r-2M}\frac{\partial^3\, {}^{(1)}K^{\text{RW}}}{\partial t^3} = 0.\end{aligned} \quad (4.83)$$

[6] In Zerilli's and Regge-Wheeler's original works, a Fourier ansatz was used for the metric perturbations, so time derivatives appeared as factors $-i\omega t$ instead of actual derivatives. Hence, this equation is referred to as being "algebraic", since it does not feature derivatives in this context.

At this point, we have a system of equations consisting of three equations of first order in r (Eqs. (4.76), (4.78) and (4.79)) and, in addition, the algebraic identity Eq. (4.83). Now we can isolate $\partial_t {}^{(1)}H_0{}^{\rm RW}$ in the algebraic identity and substitute this in Eq. (4.76) and Eq. (4.78) to obtain two coupled partial differential equations

$$\begin{aligned}\frac{\partial}{\partial r}\frac{\partial^{(1)}K^{\rm RW}}{\partial t} &= \alpha_0(r)\frac{\partial^{(1)}K^{\rm RW}}{\partial t} + \alpha_2(r)\frac{\partial^{3\,(1)}K^{\rm RW}}{\partial t^3} + \beta_0(r)\,{}^{(1)}H_1{}^{\rm RW} + \beta_2(r)\frac{\partial^{2\,(1)}H_1{}^{\rm RW}}{\partial t^2},\\ \frac{\partial}{\partial r}{}^{(1)}H_1{}^{\rm RW} &= \gamma_0(r)\frac{\partial^{(1)}K^{\rm RW}}{\partial t} + \gamma_2(r)\frac{\partial^{3\,(1)}K^{\rm RW}}{\partial t^3} + \delta_0(r)\,{}^{(1)}H_1{}^{\rm RW} + \delta_2(r)\frac{\partial^{2\,(1)}H_1{}^{\rm RW}}{\partial t^2},\end{aligned} \tag{4.84}$$

where the coefficients preceding the different time derivatives of $\partial_t {}^{(1)}K^{\rm RW}$ and ${}^{(1)}H_1{}^{\rm RW}$ can be found in `M2xS2-Split_coordinates_Final.nb` [43]. We want to decouple these equations and recast them in the form of a Schrödinger-like equation. To this end, we perform the transformation

$$\begin{aligned}\frac{\partial^{(1)}K^{\rm RW}}{\partial t} &= f(r)\,{}^{(1)}\chi(t,r) + g(r)\,{}^{(1)}\hat{R}(t,r),\\ {}^{(1)}H_1{}^{\rm RW} &= h(r)\,{}^{(1)}\chi(t,r) + k(r)\,{}^{(1)}\hat{R}(t,r),\end{aligned} \tag{4.85}$$

such that the following properties are satisfied

$$\frac{\partial^{(1)}\chi}{\partial r^*} = {}^{(1)}\hat{R}, \quad \frac{\partial^{(1)}\hat{R}}{\partial r^*} = \left[V(r^*) + \frac{\partial^2}{\partial t^2}\right]{}^{(1)}\chi, \quad \frac{\partial r}{\partial r^*} = \left(1 - \frac{2M}{r}\right). \tag{4.86}$$

The particular form of Eq. (4.86) ensures the derivatives of the wave function ${}^{(1)}\chi$ can be combined in a single Schrödinger-like equation.[7] The solution to this system, as provided in [40], is given by

$$\begin{aligned} f(r) &= \frac{\lambda(\lambda+1)r^2 + 3\lambda r + 6M^2}{r^2(\lambda r + 3M)}, & g(r) &= 1,\\ h(r) &= \frac{\lambda r^2 - 3\lambda M r - 3M^2}{(r-2M)(\lambda r + 3M)}, & k(r) &= \frac{r^2}{r-2M},\\ V(r^*) &= 2\left(1 - \frac{2M}{r}\right)\frac{\lambda^2 r^2[(\lambda+1)r + 3M] + 9M^2(\lambda r + M)}{r^3(\lambda r + 3M)^2}, \end{aligned} \tag{4.87}$$

where $\lambda \equiv \frac{1}{2}(\ell-1)(\ell+2)$. After this transformation, we have recast the linearised Einstein equations in one single equation, called the Zerilli equation:

$$\frac{\partial^{2\,(1)}\chi}{\partial {r^*}^2} - \frac{\partial^{2\,(1)}\chi}{\partial t^2} - V(r^*)\,{}^{(1)}\chi = 0, \tag{4.88}$$

which is formulated in terms of the Zerilli function ${}^{(1)}\chi$ given by

$${}^{(1)}\chi = \frac{r-2M}{\lambda r + 3M}\left[\frac{r^2}{r-2M}\frac{\partial^{(1)}K^{\rm RW}}{\partial t} - {}^{(1)}H_1{}^{\rm RW}\right]. \tag{4.89}$$

The expression for ${}^{(1)}\chi$ can be obtained by inverting the transformation in Eq. (4.85), using the solution Eq. (4.87). Alternatively, we can use the master function ${}^{(1)}\psi$ that is related to ${}^{(1)}\chi$ by

$$\frac{\partial}{\partial t}{}^{(1)}\psi = {}^{(1)}\chi, \tag{4.90}$$

[7]The aim of finding a Schrödinger-like equation is inspired by previous work of Regge and Wheeler who found a Schrödinger-like equation for the odd perturbations [39].

which equally solves the Zerilli equation. To express ${}^{(1)}\psi$ in terms of the metric perturbations, we rewrite Eq. (4.78) to be able to substitute ${}^{(1)}H_1{}^{\mathrm{RW}}$ in Eq. (4.89)

$$ {}^{(1)}\chi = \frac{2r(r-2M)}{\ell(\ell+1)(\lambda r+3M)}\left[\frac{\partial {}^{(1)}H_0{}^{\mathrm{RW}}}{\partial t} - \frac{r-3M}{r-2M}\frac{\partial {}^{(1)}K^{\mathrm{RW}}}{\partial t} - r\frac{\partial}{\partial r}\frac{\partial {}^{(1)}K^{\mathrm{RW}}}{\partial t}\right] + \frac{r^2}{\lambda r+3M}\frac{\partial {}^{(1)}K^{\mathrm{RW}}}{\partial t}, $$

such that

$$ {}^{(1)}\psi = \frac{2r(r-2M)}{\ell(\ell+1)(\lambda r+3M)}\left[{}^{(1)}H_0{}^{\mathrm{RW}} - \frac{r-3M}{r-2M}{}^{(1)}K^{\mathrm{RW}} - r\frac{\partial {}^{(1)}K^{\mathrm{RW}}}{\partial r}\right] + \frac{r^2}{\lambda r+3M}{}^{(1)}K^{\mathrm{RW}}. \tag{4.91} $$

We introduced ${}^{(1)}\psi$, because it is closely related to the master function that can be found using Moncrief's derivation [41]. This Moncrief wave function ${}^{(1)}\psi_{\mathrm{Mon}}$ is gauge invariant and defined solely in terms of the components of the spatial metric γ_{ab}. It reads

$$ {}^{(1)}\psi_{\mathrm{Mon}} = \frac{2(r-2M)}{\ell(\ell+1)(\lambda r+3M)}\left[r\,{}^{(1)}H_2 + 3r^2\frac{\partial {}^{(1)}G}{\partial r} - \frac{r-3M}{r-2M}{}^{(1)}K - r^2\frac{\partial {}^{(1)}K}{\partial r} - 6\,{}^{(1)}h_1\right] + \frac{r^2}{\lambda r+3M}{}^{(1)}K, \tag{4.92} $$

where any arbitrary gauge can be used for the Regge-Wheeler perturbations. When we compare this to our expression for ${}^{(1)}\psi$ in Eq. (4.91), it is apparent that our expression is simply the Moncrief function specifically evaluated in the Regge-Wheeler gauge.

At first order, we will use the Moncrief function Eq. (4.92) as our master function, since it is already tailored for using initial data. Furthermore, due to its gauge invariance, we can simply insert the components of ${}^{(1)}\gamma''{}_{ab}$ in the gauge we have specified before.

As a side note, we also observe that we can express all the metric perturbations ${}^{(1)}K^{\mathrm{RW}}$, ${}^{(1)}H_1{}^{\mathrm{RW}}$ and ${}^{(1)}H_0{}^{\mathrm{RW}}$ in the RW gauge in terms of the Moncrief function. The transformation in Eq. (4.85) and Eq. (4.86), can thus be rewritten as

$$ {}^{(1)}K^{\mathrm{RW}} = f(r)\,{}^{(1)}\psi + \left(1-\frac{2M}{r}\right)\frac{\partial {}^{(1)}\psi}{\partial r}, \tag{4.93} $$

$$ {}^{(1)}H_1{}^{\mathrm{RW}} = h(r)\frac{\partial {}^{(1)}\psi}{\partial t} + r\frac{\partial^2\,{}^{(1)}\psi}{\partial r\partial t}, \tag{4.94} $$

$$ {}^{(1)}H_0{}^{\mathrm{RW}} = \frac{\partial}{\partial r}\left[\left(1-\frac{2M}{r}\right)h(r)\,{}^{(1)}\psi + r\frac{\partial {}^{(1)}\psi}{\partial r}\right] - {}^{(1)}K^{\mathrm{RW}}, \tag{4.95} $$

where we used Eq. (4.76) to derive the expression for ${}^{(1)}H_0{}^{\mathrm{RW}}$.

Because the $\ell = 0$ mode of γ_{ab} is non-radiative (and even set to zero in our case), we are only interested in the $\ell = 2$ modes. Hence, the initial master function that wel will plug into the Zerilli equation will be

$$ {}^{(1)}\psi^{(\ell=2)} = \frac{r-2M}{3(2r+3M)}\left[r\,{}^{(1)}H_2{}^{(\ell=2)} + 3r^2\frac{\partial {}^{(1)}G^{(\ell=2)}}{\partial r} - r^2\frac{\partial {}^{(1)}K^{(\ell=2)}}{\partial r} - 6\,{}^{(1)}h_1{}^{(\ell=2)}\right] - \frac{r}{3}{}^{(1)}K^{(\ell=2)}. \tag{4.96} $$

We also need to supply the initial time derivative of ${}^{(1)}\psi^{(\ell=2)}$, to make our initial value problem well-defined. Note that we are working in a gauge such that ${}^{(1)}H_0 = {}^{(1)}H_1 = {}^{(1)}h_0 = 0$ for the quadrupolar modes, which implies that time derivatives of the metric can easily be related to the extrinsic curvature via Eq. (2.20). Therefore, the time derivative $\partial_t {}^{(1)}\psi^{(\ell=2)}$ can be expressed in terms of curvature perturbations as

$$\begin{aligned}\partial_t {}^{(1)}\psi^{(\ell=2)} =& \frac{2(r-2M)^{3/2}}{3\sqrt{r}(2r+3M)}\left[{}^{(1)}KH_2{}^{(\ell=2)} + 3r\frac{\partial^{(1)}KG^{(\ell=2)}}{\partial r} - r\frac{\partial^{(1)}KK^{(\ell=2)}}{\partial r} - \tfrac{6}{r}{}^{(1)}Kh_1{}^{(\ell=2)}\right] \\ &- \frac{2\sqrt{r-2M}}{3\sqrt{r}}{}^{(1)}KK^{(\ell=2)}.\end{aligned} \tag{4.97}$$

In [25], they have found the particularly easy form

$$\partial_t {}^{(1)}\psi^{(\ell=2)} = \frac{2\sqrt{r-2M}}{\sqrt{r}(2r+3M)}\left[-r(2M-r){}^{(1)}KG^{(\ell=2)} - r^{2\,(1)}KK^{(\ell=2)} + (r-2M){}^{(1)}Kh_1{}^{(\ell=2)}\right],$$

by using the first order Einstein equations to simplify higher order time derivatives. It is not clear whether they take the time derivative ${}^{(1)}\psi^{(\ell=2)}$ or ${}^{(1)}\psi^{(\ell=2)}$ itself as the starting point. We have not been able to reproduce this expression, so we will stick to Eq. (4.97).

Filling in the explicit initial data for the BHs in a head-on collission in Eq. (4.62), we find the function

$${}^{(1)}\psi^{(\ell=2)}\big|_{t=0} = \frac{8L^2Mr\left(7\sqrt{r(r-2M)} - 10M + 5r\right)}{3\sqrt{r-2M}(3M+2r)\left(\sqrt{r-2M}+\sqrt{r}\right)^5}, \tag{4.98}$$

and from the initial extrinsic curvature perturbations in Eqs. (4.63)–(4.65), we obtain the time derivative

$$\partial_t {}^{(1)}\psi^{(\ell=2)}\big|_{t=0} = -\frac{2LP\sqrt{r-2M}(19M+8r)}{3r^{7/2}(3M+2r)}. \tag{4.99}$$

Note that since ${}^{(1)}H_0^{(\ell=0)}$ is the only non-vanishing $\ell=0$ perturbation, both ${}^{(1)}\psi^{(\ell=0)}|_{t=0}$ and $\partial_t {}^{(1)}\psi^{(\ell=0)}|_{t=0}$ vanish. The results for ${}^{(1)}\psi^{(\ell=2)}|_{t=0}$ and $\partial_t {}^{(1)}\psi^{(\ell=2)}|_{t=0}$, we have obtained here, both agree with [25]. This was to be expected as we found the same first order metric perturbations.

4.4.2 Second Order

We proceed with the second order calculation. The derivation is essentially the same. We start from the Einstein equations again, but now from Eq. (2.24). We simply replace all (1) superscripts by (2) for the equations generated by $\delta R_{\mu\nu}[{}^{(2)}g]$. The terms $\delta^2 R_{\mu\nu}[{}^{(1)}g, {}^{(1)}g]$ give rise to additional quadratic terms which we will refer to as source terms denoted by some S. Repeating the same calculations will ultimately result in a Zerilli equation for the second order perturbations that has a source term quadratic in the first order perturbations.

Before we can begin with the second order derivation, we have to pay attention to a problem: the non-uniqueness of second order gauge choices. Recall that at second order the gauge choice depends on the choice made at first order. For the following calculations, we only need to choose the 2nd order Regge-Wheeler gauge ${}^{(2)}G = {}^{(2)}h_0 = {}^{(2)}h_1 = 0$. We are free to choose any first order gauge, which would result in different source terms. We will also select the RW gauge at first order, in order to have more manageable, condensed source terms. We will explicitly indicate this first order gauge condition by adding a RW subscript to the quadratic terms.

We start by decomposing the second order Einstein equation Eq. (2.24), into Legendre polynomials. Given that we are dealing with the product of different modes of tensorial harmonics, it neither easy nor practical to give general expressions. Since the $\ell = 2$ is the only radiative mode we have taken into consideration, we will only consider the quadratic terms that contribute to the source term for the $\ell = 2$ wave function. The quadratic first order modes $(\ell = 0) \times (\ell = 2)$, $(\ell = 0) \times (\ell = 2)$ and $(\ell = 2) \times (\ell = 2)$ will all contribute to the source term. To keep the expressions somewhat manageable we will only present the contributions of the $(\ell = 2) \times (\ell = 2)$ mode in print, but the full calculations in `M2xS2-Split_Coordinates_Final.nb` take all terms into account [43].

Our starting point is the RW gauge ${}^{(2)}G = {}^{(2)}h_0 = {}^{(2)}h_1 = 0$. As already mentioned, we make the additional assumption that at first order the RW gauge is also satisfied. The decomposition of $\delta R_{\mu\nu}[{}^{(2)}g]$ in this gauge is given by Eqs. (C.28)–(C.30) and the one for $\delta^2 R_{\mu\nu}[{}^{(1)}g, {}^{(1)}g]$ can be found in Eqs. (C.31)–(C.33). Similar to the first order derivation, we obtain an algebraic relation between ${}^{(2)}{H_2}^{\mathrm{RW}}$ and ${}^{(2)}{H_0}^{\mathrm{RW}}$ given by

$$ {}^{(2)}{H_2}^{\mathrm{RW}} = {}^{(2)}{H_0}^{\mathrm{RW}} + S^{\mathrm{RW}}_{H_2}, \tag{4.100} $$

which now has an additional source term $S^{\mathrm{RW}}_{H_2}$, named after the LHS of the equation. We also suppressed the $(\ell = 2)$ label for the second order perturbations. We will continue to do this for the remainder of this section. When we replace ${}^{(2)}{H_2}^{\mathrm{RW}}$ by ${}^{(2)}{H_0}^{\mathrm{RW}}$, using Eq. (4.100), this will introduce additional quadratic terms. Like the first order calculations, we also obtain a system of three first order equations in r:

$$ \frac{\partial\, {}^{(2)}{H_1}^{\mathrm{RW}}}{\partial r} = \frac{r}{r-2M}\frac{\partial\, {}^{(2)}{H_0}^{\mathrm{RW}}}{\partial t} + \frac{r}{r-2M}\frac{\partial\, {}^{(2)}K^{\mathrm{RW}}}{\partial t} - \frac{2M}{r\,(r-2M)}\,{}^{(2)}{H_1}^{\mathrm{RW}} + S^{\mathrm{RW}}_{H_{1,r}}, \tag{4.101} $$

$$ \frac{\partial^2\, {}^{(2)}K^{\mathrm{RW}}}{\partial t \partial r} = \frac{1}{r}\frac{\partial\, {}^{(2)}{H_0}^{\mathrm{RW}}}{\partial t} + \frac{\ell(\ell+1)}{2r^2}\,{}^{(2)}{H_1}^{\mathrm{RW}} - \frac{r-3M}{r\,(r-2M)}\frac{\partial\, {}^{(2)}K^{\mathrm{RW}}}{\partial t} + S^{\mathrm{RW}}_{K_{,t,r}}, \tag{4.102} $$

$$ \begin{aligned} \frac{\partial^2\, {}^{(2)}{H_0}^{\mathrm{RW}}}{\partial t \partial r} = &\frac{r}{r-2M}\frac{\partial^2\, {}^{(2)}{H_1}^{\mathrm{RW}}}{\partial t^2} + \frac{r-4M}{r\,(r-2M)}\frac{\partial\, {}^{(2)}{H_0}^{\mathrm{RW}}}{\partial t} - \frac{r-3M}{r\,(r-2M)}\frac{\partial\, {}^{(2)}K^{\mathrm{RW}}}{\partial t} \\ &+ \frac{\ell(\ell+1)}{2r^2}\,{}^{(2)}{H_1}^{\mathrm{RW}} + S^{\mathrm{RW}}_{H_{0,t,r}}, \end{aligned} \tag{4.103} $$

which have also been amended by some source terms, named after the derivative on the LHS of the equation. Furthermore, the set consisting of three second order differential equations in r can once more be rewritten as the "algebraic identity"

$$ \begin{aligned} &-\frac{\ell(\ell+1)M}{r^2}\,{}^{(2)}{H_1}^{\mathrm{RW}} - 2r\frac{\partial^2\, {}^{(2)}{H_1}^{\mathrm{RW}}}{\partial t^2} - \left[(\ell-1)(\ell+1) + \frac{6M}{r^2}\right]\frac{\partial\, {}^{(2)}{H_0}^{\mathrm{RW}}}{\partial t} \\ &+ \left[(\ell+2)(\ell-1) + \frac{2M(r-3M)}{r(r-2M)}\right]\frac{\partial\, {}^{(2)}K^{\mathrm{RW}}}{\partial t} + \frac{2r^3}{r-2M}\frac{\partial^3\, {}^{(2)}K^{\mathrm{RW}}}{\partial t^3} + S^{\mathrm{RW}}_{\mathrm{alg}} = 0. \end{aligned} \tag{4.104} $$

Most of the source terms are long and tedious expression that would not be very illuminating to present in print. The full calculations including the source terms can be found in the `M2xS2-Split_Coordinates_Final.nb` notebook [43]. There are two source terms that are practical to discuss, since they are quite short and can be compared to the literature [14]. The first of them is the source term that enters in the algebraic relation between ${}^{(2)}{H_2}^{\mathrm{RW}}$ and ${}^{(2)}{H_0}^{\mathrm{RW}}$. The contributions as a consequence of $(\ell = 2) \times (\ell = 2)$ are given by

$$ S^{\mathrm{RW},(2)\times(2)}_{H_2} = \frac{83}{35}\left[({}^{(1)}{H_1}^{\mathrm{RW}})^2 - ({}^{(1)}{H_0}^{\mathrm{RW}})^2\right], $$

where we have dropped the ($\ell = 2$) labels for the first order quantities on the RHS. This exhibits the same form as in [14], the only difference being the factor 83/35 instead of 1/7. The second one is the source term that follows from the tB-component of the Einstein equations, provided in Eq. (4.101). Here, we find the source term

$$S_{H_1}^{\mathrm{RW},(2)\times(2)} = -\frac{r}{70(r-2M)}\frac{\partial}{\partial t}\left[10({}^{(1)}K^{\mathrm{RW}})^2 + 171({}^{(1)}H_0{}^{\mathrm{RW}})^2 - 171({}^{(1)}H_1{}^{\mathrm{RW}})^2\right],$$

where we dropped the ($\ell = 2$) label for the first order perturbations. Again we find the same form as in [14], but instead of the factor 2/14, 3/14 and −3/14, respectively, we find 1/7, 171/70 and −171/70. It has to be remarked that these factors also depend on the factors present in $S_{H_2}^{\mathrm{RW}}$, as a consequence of the substitution of ${}^{(2)}H_2{}^{\mathrm{RW}}$.

Now we continue like we did at first order and eliminate $\partial_t {}^{(2)}H_0{}^{\mathrm{RW}}$ from Eqs. (4.101) and (4.102) using the algebraic identity, Eq. (4.104). This yields a set of two coupled differential equations, similar to Eq. (4.84). Namely,

$$\begin{aligned}\frac{\partial}{\partial r}\frac{\partial {}^{(2)}K^{\mathrm{RW}}}{\partial t} &= \alpha_0(r)\frac{\partial {}^{(2)}K^{\mathrm{RW}}}{\partial t} + \alpha_2(r)\frac{\partial^3 {}^{(2)}K^{\mathrm{RW}}}{\partial t^3} + \beta_0(r)\,{}^{(2)}H_1{}^{\mathrm{RW}} + \beta_2(r)\frac{\partial^2 {}^{(2)}H_1{}^{\mathrm{RW}}}{\partial t^2} + S_1^{\mathrm{RW}},\\ \frac{\partial}{\partial r}{}^{(2)}H_1{}^{\mathrm{RW}} &= \gamma_0(r)\frac{\partial {}^{(2)}K^{\mathrm{RW}}}{\partial t} + \gamma_2(r)\frac{\partial^3 {}^{(2)}K^{\mathrm{RW}}}{\partial t^3} + \delta_0(r)\,{}^{(2)}H_1{}^{\mathrm{RW}} + \delta_2(r)\frac{\partial^2 {}^{(2)}H_1{}^{\mathrm{RW}}}{\partial t^2} + S_2^{\mathrm{RW}},\end{aligned} \tag{4.105}$$

where the coefficients $\alpha_0(r), \alpha_2(r), \ldots$ are the same as in the first order calculations. This system can be transformed into a Schrödinger-like equation by imposing the transformation

$$\begin{aligned}\frac{\partial {}^{(2)}K^{\mathrm{RW}}}{\partial t} &= f(r)\,{}^{(2)}\chi(t,r) + g(r)\,{}^{(2)}\hat{R}(t,r),\\ {}^{(2)}H_1{}^{\mathrm{RW}} &= h(r)\,{}^{(2)}\chi(t,r) + k(r)\,{}^{(2)}\hat{R}(t,r),\end{aligned} \tag{4.106}$$

such that the following relations are satisfied by ${}^{(2)}\chi$ and ${}^{(2)}\hat{R}$:

$$\frac{\partial {}^{(2)}\chi}{\partial r^*} = {}^{(2)}\hat{R} + S_\chi^{\mathrm{RW}}, \quad \frac{\partial {}^{(2)}\hat{R}}{\partial r^*} = \left[V(r^*) + \frac{\partial^2}{\partial t^2}\right]{}^{(2)}\chi + S_{\hat{R}}^{\mathrm{RW}}, \quad \frac{\partial r}{\partial r^*} = \left(1 - \frac{2M}{r}\right). \tag{4.107}$$

This yields the same set of equations for $f(r), g(r), h(r), k(r)$ and $V(r^*)$ that is solved by the expressions in (4.87) once more. Hence, we find the same expressions for ${}^{(2)}\chi$ and ${}^{(2)}\hat{R}$, but with all first order quantities simply replaced by second order ones. By applying an r^* derivative to ${}^{(2)}\chi$ and simplifying higher order derivatives with Eq. (4.105), a comparison to the expression for ${}^{(2)}\hat{R}$ yields the source term

$$\begin{aligned}S_\chi^{\mathrm{RW},(2)\times(2)} =& \frac{r-2M}{7(2r+3M)}\Bigg(2\,{}^{(1)}H_1{}^{\mathrm{RW}}\partial_r {}^{(1)}H_0{}^{\mathrm{RW}} - r\partial_r {}^{(1)}H_0{}^{\mathrm{RW}}\partial_t {}^{(1)}K^{\mathrm{RW}} + r\partial_r {}^{(1)}K^{\mathrm{RW}}\partial_t {}^{(1)}H_0{}^{\mathrm{RW}}\\ &+ r\partial_r {}^{(1)}K^{\mathrm{RW}}\partial_t {}^{(1)}K^{\mathrm{RW}} + 2r\,{}^{(1)}K^{\mathrm{RW}}\partial_t\partial_r {}^{(1)}K^{\mathrm{RW}} + (r-2M)\,{}^{(1)}H_1{}^{\mathrm{RW}}\partial_r^2 {}^{(1)}H_0{}^{\mathrm{RW}}\\ &- {}^{(1)}H_0{}^{\mathrm{RW}}\partial_t {}^{(1)}H_1{}^{\mathrm{RW}} + \frac{4r-10M}{r-2M}{}^{(1)}K^{\mathrm{RW}}\partial_t {}^{(1)}K^{\mathrm{RW}} + \frac{8M^2+8Mr-6r^2}{r^2(r-2M)}{}^{(1)}H_1{}^{\mathrm{RW}}\,{}^{(1)}K^{\mathrm{RW}}\\ &- \frac{2M}{r}{}^{(1)}H_1{}^{\mathrm{RW}}\partial_r {}^{(1)}K^{\mathrm{RW}} - \frac{r}{r-2M}{}^{(1)}H_1{}^{\mathrm{RW}}\partial_t {}^{(1)}H_1{}^{\mathrm{RW}}\\ &- \frac{2}{r}{}^{(1)}H_1{}^{\mathrm{RW}}\partial_t\partial_r {}^{(1)}H_1{}^{\mathrm{RW}} + \frac{r^2}{r-2M}{}^{(1)}H_1{}^{\mathrm{RW}}\partial_t^2 {}^{(1)}H_0{}^{\mathrm{RW}}\Bigg),\end{aligned}$$

where ($\ell = 2$) superscripts have again been suppressed for notational clarity. This source term does not agree with the source term in Eq. (10) of [14], which has fewer terms than our expression. The general form tends to be the same, but due to some different coefficients we seem to have obtained slightly different coefficients here and there. Using a similar approach as for S_χ^{RW}, we are able to determine $S_{\hat{R}}^{\mathrm{RW}}$. We can now combine the source terms in Eq. (4.107) as a single source term S_{RW}[8], and write the second order Zerilli equation as

$$\frac{\partial^2\, {}^{(2)}\chi^{(\ell=2)}}{\partial r^{*2}} - \frac{\partial^2\, {}^{(2)}\chi^{(\ell=2)}}{\partial t^2} - V(r^*)\, {}^{(2)}\chi = S_{\mathrm{RW}}, \tag{4.108}$$

where the source term satisfies

$$S_{\mathrm{RW}} = \left(1 - \frac{2M}{r}\right)\frac{\partial S_\chi^{\mathrm{RW}}}{\partial r} + S_{\hat{R}}^{\mathrm{RW}}.$$

The source term S_{RW} is a lengthy expression in terms of ${}^{(1)}H_0{}^{\mathrm{RW}}$, ${}^{(1)}H_1{}^{\mathrm{RW}}$ and ${}^{(1)}K^{\mathrm{RW}}$. To make it somewhat more compact, we can relate the perturbations in the RW gauge to ${}^{(1)}\psi^{(\ell)}$ via Eq. (4.93)–(4.95). This allows us to express the source term S_{RW} in terms of derivatives of ${}^{(1)}\psi^{(\ell)}$. The source term contains higher order time derivatives of ${}^{(1)}\psi^{(\ell)}$, but the order of these time derivatives can be reduced. Since ${}^{(1)}\psi^{(\ell)}$ satisfies the first order Zerilli equation, double time derivatives can be substituted for r derivatives. Consequently, the source term can be written fully in terms of ${}^{(1)}\psi^{(\ell)}$ and $\partial_t\, {}^{(1)}\psi^{(\ell)}$, and their r derivatives. After these simplifications, S_{RW} is still too lengthy to represent in print. For the full expression we refer to `M2xS2-Split_Coordinates_Final.nb` [43].

By substituting the expression for ${}^{(1)}\psi^{(\ell)}|_{t=0}$ and $\partial_t\, {}^{(1)}\psi^{(\ell)}|_{t=0}$ into S^{RW}, we can determine the initial source term. It consists of a L^4, L^3P and L^2P^2 contributions. Note that, in this case, the $\ell = 0$ modes do not contribute to the source term, since ${}^{(1)}\psi^{\ell=0}|_{t=0} = 0$ and $\partial_t\, {}^{(1)}\psi^{\ell=0}|_{t=0} = 0$ as discussed before. Thus, we only have ($\ell = 2$) contributions. The analytical results are once more to cumbersome to fully display here. The algebraic expression can be found in `M2xS2-Split_Coordinates_Final.nb` [43]. A plot of the different contributions is presented in Fig. 9. Each contribution is maximal near the horizon.

The second order wave function ${}^{(2)}\chi$ can be determined by inverting Eq. (4.106). This yields the familiar result

$${}^{(2)}\chi = \frac{r-2M}{\lambda r + 3M}\left[\frac{r^2}{r-2M}\frac{\partial\, {}^{(2)}K^{\mathrm{RW}}}{\partial t} - {}^{(2)}H_1{}^{\mathrm{RW}}\right]. \tag{4.109}$$

Note that now that a source term is present, there is no straightforward relation between the Zerilli function ${}^{(2)}\chi$ and Moncrief function ${}^{(2)}\psi$ anymore. We will elaborate on using ${}^{(2)}\psi$ at the end of this section. For now, we will use ${}^{(2)}\chi$ as the master function at second order.

To determine its initial value, we will treat the metric perturbations in the RW gauge as a shorthand for the gauge invariant combinations again. In this context, gauge invariant means invariant under a *pure* second order transformation. This means we can just use Eqs. (C.24)–(C.27), where we simply replace everything by its second order counterpart. If at second order the perturbations satisfy ${}^{(2)}H_0 = {}^{(2)}H_1 = {}^{(2)}h_0 = 0$, this can be specified in terms of the initial perturbations by replacing the time derivatives by extrinsic curvature

[8] This source term is not to be confused with $\mathcal{S}_{\mathrm{RW}}$ in [46], which is obtained from a different derivation based on Moncrief's gauge invariant approach.

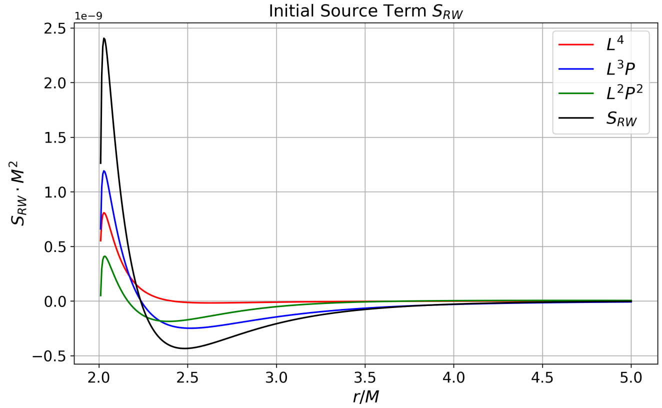


Figure 9: Plot of the initial source term S_{RW}. The L^4, L^3P and L^2P^2 contributions are plotted separately in red, blue and green, respectively. For this plot the values $M = 1$, $P = 0.01$ and $L = 0.01$ were used.

perturbations, using Eq. (2.20). This yields

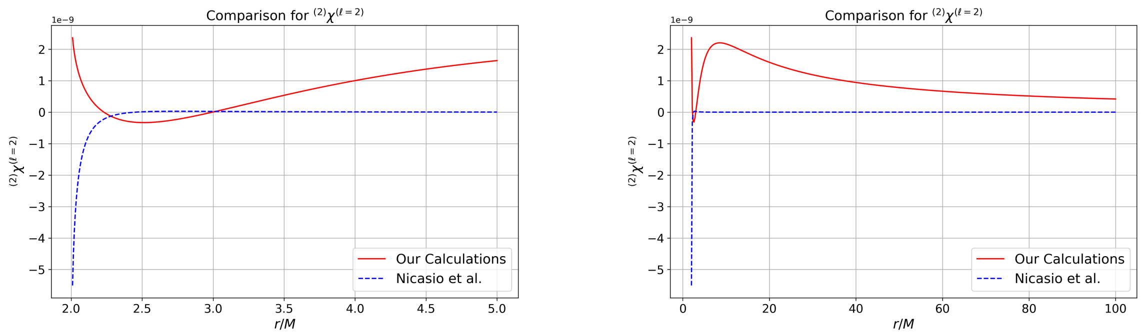
$$\begin{aligned}\frac{\partial^{(2)}K^{\mathrm{RW}}}{\partial t} =&2\sqrt{1-\frac{2M}{r}}\left[{}^{(2)}KK - \frac{2}{r}\left(1-\frac{2M}{r}\right)\left[{}^{(2)}Kh_1 - \frac{r^2}{2}\frac{\partial^{(2)}G}{\partial r}\right]\right],\\ {}^{(2)}H_1{}^{\mathrm{RW}} =&-2\sqrt{1-\frac{2M}{r}}\,{}^{(1)}Kh_1 + \frac{\sqrt{r}(r-3M)}{\sqrt{r-2M}}\,{}^{(1)}KG + 4r^2\sqrt{1-\frac{2M}{r}}\frac{\partial^{(1)}KG}{\partial r}.\end{aligned}$$

Note that in our calculations, the condition ${}^{(2)}H_0 = {}^{(2)}H_1 = {}^{(2)}h_0 = 0$ is indeed satisfied. Hence, we can determine $\partial_t{}^{(2)}K^{\mathrm{RW}}|_{t=0}$ and ${}^{(2)}H_1{}^{\mathrm{RW}}|_{t=0}$ from our set of initial metric and extrinsic curvature perturbations. The resulting expressions are too long to present in print but both scale with L^3P. As a consequence, the resulting initial wave function ${}^{(2)}\chi|_{t=0}$ also scales with P^3L. For the full analytical expressions, we refer to `M2xS2-Split_Coordinates_Final.nb` [43]. Note that we do not only get a far more complicated term for ${}^{(2)}\chi|_{t=0}$ compared to [25], we also have different scaling behaviour since we lack a term that scales with L^4. The comparison of the initial wave functions can be found in Fig. 10. It is clear that both functions show different behaviour. For [25], the negative L^4 term is dominant near the horizon, while in our case the logarithms in the L^3P term are dominant. The two expressions do, however, both converge to 0 for large r, albeit our expression does so at a much slower pace.

We also need to specify the initial time derivative of the Zerilli function $\partial_t{}^{(2)}\chi|_{t=0}$. Starting from Eq. (4.109), one finds

$$\partial_t{}^{(2)}\chi = \frac{r-2M}{\lambda r + 3M}\left[\frac{r^2}{r-2M}\frac{\partial^{2\,(2)}K^{\mathrm{RW}}}{\partial t^2} - \frac{\partial^{(2)}H_1{}^{\mathrm{RW}}}{\partial t}\right].$$

We need to eliminate the time derivatives to make sure everything can be determined in terms of the initial metric and extrinsic curvature perturbations, which only cover the zeroth and first order time derivatives, respectively. This can be accomplished by using the Einstein equations to determine the time derivatives in terms of lower order time derivatives. We can determine $\partial_t{}^{(2)}H_1{}^{\mathrm{RW}}$ using the rB-component of the Einstein equations and we can determine $\partial_t{}^{(2)}K^{\mathrm{RW}}$ by using the differential equation that follows from the



(a) Plot of $^{(2)}\chi^{(\ell=2)}$ for $r \in (2M, 5M)$.

(b) Plot of $^{(2)}\chi^{(\ell=2)}$ for $r \in (2M, 100M)$.

Figure 10: Comparison of the different expressions for $^{(2)}\chi^{(\ell=2)}$ from our calculations (red) and from [25] (blue). The functions are plotted for $M = 1$, $P = 0.01$ and $L = 0.01$. Note both functions diverge at the horizon and both converge to 0 at infinity.

AB-component. This provides the relations

$$\frac{\partial {}^{(2)}{H_1}^{\text{RW}}}{\partial t} = \frac{r-2M}{r}\left[\frac{\partial {}^{(2)}{H_0}^{\text{RW}}}{\partial r} - \frac{\partial {}^{(2)}K^{\text{RW}}}{\partial r}\right]\frac{2M}{r^2}{}^{(2)}{H_0}^{\text{RW}} + S^{\text{RW}}_{H_1,t}, \tag{4.110}$$

$$\frac{\partial^2 {}^{(2)}K^{\text{RW}}}{\partial t^2} = \frac{2}{r(r-2M)}{}^{(2)}{H_0}^{\text{RW}} + \frac{2}{r}\frac{\partial {}^{(2)}{H_0}^{\text{RW}}}{\partial r} - \frac{2}{r-2M}\frac{\partial {}^{(2)}{H_1}^{\text{RW}}}{\partial t} \tag{4.111}$$

$$+ \frac{(\ell+2)(\ell-1)}{r(r-2M)}{}^{(2)}K^{\text{RW}} - \frac{4r-6M}{r(r-2M)}\frac{\partial {}^{(2)}K^{\text{RW}}}{\partial r} + \frac{r^2}{(r-2M)^2}\frac{\partial^2 {}^{(2)}K^{\text{RW}}}{\partial r^2} + S^{\text{RW}}_{K,t,t}, \tag{4.112}$$

where the source terms are once again named after the derivatives on the LHS. Note we can substitute the expression in Eq. (4.110) for $\partial {}^{(2)}{H_1}^{\text{RW}}$ in Eq. (4.112) to eliminate all time derivatives. Furthermore, we can apply the same treatment to the source terms $S^{\text{RW}}_{H_1,t}$ and $S^{\text{RW}}_{K,t,t}$ as we applied to S_{RW}: we replace the perturbations in the RW-gauge by derivatives of $^{(1)}\psi^{(\ell)}$, eliminate higher order derivatives using the Zerilli equation and substitute the expressions for $^{(1)}\psi^{(\ell=2)}|_{t=0}$ and $^{(1)}\psi^{(\ell=2)}|_{t=0}$. This enables us to determine everything in terms of the initial data we calculated in Sec. 4. The final expressions can be found in `M2xS2-Split_Coordinates_Final.nb` [43], where we find an L^4, L^3P and L^2P^2 term. The comparison to the expressions in [25] are plotted in Fig. 11. Again, the results differ near the horizon, but both expressions converge to the value 0 at spatial infinity.

The calculation of the initial wave function and its derivative would have been more straightforward, without have to resort to Einstein equations, if we were to have a second order equivalent of the Moncrief function. This wave function would be first and second order gauge invariant under the full gauge transformation and would be defined in terms of solely the initial data, meaning we do not have to reduce time derivatives. However, we have to take two things into account to set up the second order evolution for such a master function. First, the Moncrief function $^{(2)}\psi$ will satisfy a different equation than the Zerilli function $^{(2)}\chi$ due to the source term [46]. The evolution for $^{(2)}\psi$ will be described by the Zerilli equation

$$\frac{\partial^2 {}^{(2)}\psi}{\partial {r^*}^2} - \frac{\partial^2 {}^{(2)}\psi}{\partial t^2} - V(r^*)^{(2)}\psi = S_{\text{Mon}}, \tag{4.113}$$

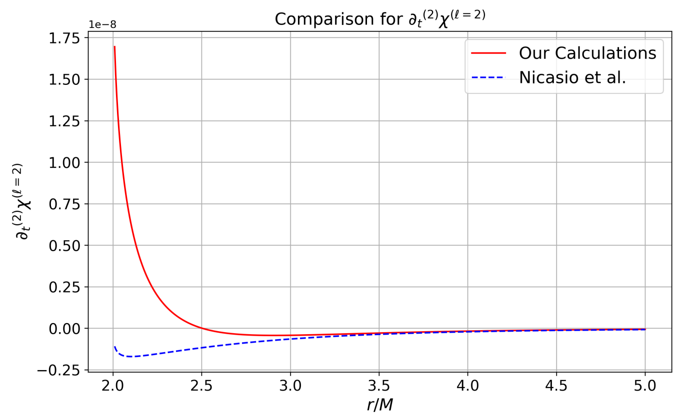


Figure 11: Comparison of the expressions for $\partial_t{}^{(2)}\chi$ from our calculations (red) and [25] (blue). The plots were generated for values $M = 1$, $P = 0.01$, $L = 0.01$ and $q_2 = 0.224 \cdot 2/M$.

where S_{Mon} is the source term that one would obtain by repeating Moncrief's derivation in [41] at second order by carefully bookkeeping the quadratic terms. Second, the wave function ${}^{(2)}\psi$ which is the second order equivalent of Eq. (4.92) is only gauge invariant under second order transformations. A first order transformation, nevertheless, will result in all sorts of quadratic terms that violate gauge invariance (see App. C.1). Hence, we will have to amend the Moncrief function with an additional term ${}^{(1)}Q$ to ${}^{(2)}\Psi \equiv {}^{(2)}\psi + {}^{(1)}Q$ that negates all the quadratic terms that appear as a consequence of the first order transformation of ${}^{(2)}\psi$ [46]. The additional term ${}^{(1)}Q$ will also change the source term, since the Zerilli equation works on it. This will ultimately result in the Zerilli equation for ${}^{(2)}\Psi$ with source term S_Ψ. We have not carried out these calculations in this work.

5 Outlook

To summarise, we established the CLA for a binary of two momentarily static BHs and a BBH in a head-on collission with small initial momentum. Due to the convenient analytical form of the BL initial data, treating these systems as perturbations of a Schwarzschild background was straightforward. The static system was covered up to first order as an example. Our primary focus was the head-on collision and the analysis for this BBH was conducted up to second order. We began by setting up the initial data, using BY initial data. Then, we extracted the perturbations, consisting of even-parity first and second order specifically examining the $\ell = 0$ and $\ell = 2$ pieces. Next, we applied gauge transformations to eliminate $\ell = 0$ contributions at first order and set $H_0 = H_1 = h_0 = 0$ at second order. Finally, we concluded by deriving the Zerilli Equations and corresponding wave functions for the $\ell = 2$ modes at both orders, including the source term at second order. Our first first order calculations were consistent with the literature [25], but at second order we encountered some differences, such as more complicated expressions for perturbations, ${}^{(1)}H_0^{(\ell=0)}$ not vanishing after the first order gauge transformation and a considerably lengthier source term.

Up to this point, we have focused exclusively on the analytical aspect of the calculations involved in the CLA. However, numerical integration is an essential component of the overall process. The initial wave functions derived thus far offer limited insight. Only through numerical integration do we obtain a full spacetime, for which we can begin to make meaningful predictions and analyse the physical characteristics of the system. So, after the subsequent numerical integration substantive results will emerge.

The numerical solver has to solve a set of two coupled partial differential equations: the solution ${}^{(1)}\psi$ to the first order Zerilli equation will serve as a source term in the Zerilli equation for the second order wave function ${}^{(2)}\chi$. This warrants a two-step approach where, in each integration step, we first extrapolate ${}^{(1)}\psi|_t$ by integrating the first order Zerilli equation. Subsequently, we update the second order Zerilli equation by modifying the source term with the newly obtained ${}^{(1)}\psi|_{t+dt}$. Finally ${}^{(2)}\chi|_{t+dt}$ can be determined by integrating the updated Zerilli equation.

The source term presents additional challenges during numerical integration. In its current form, the source term is divergent, which impedes proper convergence of the numerical solver. The divergence of the source term does not indicate a physical singularity, but is instead an artefact of the particular gauge choice [14, 16]. There are two ways to circumvent this problem that are both related to the fact that the second order Zerilli equation is not unique. First, note that the second order RW gauge depends on the first order gauge choice. One approach is to switch to a different first order gauge and repeat the derivation to obtain a Zerilli equation with an alternative source term. This gauge can be chosen such that the source term does not suffer from divergences. In the asymptotically flat gauge, for instance, perturbations remain finite at spatial infinity. The second approach turns out to be far easier. We can also modify the source term by redefining a "renormalised" wavefunction ${}^{(2)}\chi_{\text{ren}} = {}^{(2)}\chi + {}^{(1)}Q$, where ${}^{(1)}Q$ is some term quadratic in the first order perturbations. In the work of Gleiser and collaborators they take

$$ {}^{(2)}\chi_{\text{ren}} = {}^{(2)}\chi - \frac{2}{7}\left[\frac{r^2}{2r+3M}\,{}^{(1)}K^{\text{RW}}\frac{\partial\,{}^{(1)}K^{\text{RW}}}{\partial t} + ({}^{(1)}K^{\text{RW}})^2\right]. $$

This leads to the renormalised source term $\mathcal{S}_{\text{ren}}$ in the RW gauge as presented in Eq. (18) of [22]. This aspect requires further investigation for our own calculations.

With a well-behaved numerical solver, we can finally examine the physics of the BBH. A first important consistency check would involve comparing the gravitational wave signal predicted by our model to the waveform from Nicasio *et al.* [25] and to a NR simulation for a head-on collision from the RIT catalogue [47], for example. It is also valuable to determine the range of initial separations L for which agreement with NR simulations is maintained, thus assessing the extent to which we can apply the CLA. Previous publications suggest a surprising degree of accuracy for only moderately small L [5, 16, 17].

After we have determined the radiated GWs, it is possible to verify whether quadratic QNMs are indeed present in the ringdown phase as predicted by NR simulations [2, 48]. Given that the $(\ell = 2, m = 0, n = 0)$ mode with frequency ω_{200} is dominant a first order, the $(2, 0, 0) \times (2, 0, 0)$ mode with frequency $2\omega_{200}$ is expected to be the dominant quadratic mode. This mode appears most evidently in the source term for ${}^{(i)}\chi^{(\ell=4)}$. Consequently, it is necessary to revisit the calculations in Sec. 4, now incorporating the $\ell = 4$ terms. The analysis can be readily adapted to include $\ell = 4$ modes. For instance, we have already calculated the $\ell = 4$ contribution for $\hat{K}_{ab}$ and ϕ_{reg}. In Sec. 4.2, it is straightforward to calculate the $\ell = 4$ modes for γ_{ab} from Eq. (4.23) and for K_{ab} from Eq. (4.30). The approach to the first order gauge transformation will remain unchanged since it only involves $\ell = 0$ modes. For the second order transformation, one would also need to calculate ${}^{(2)}\xi^{(\ell=4)}$. Extending the remaining analysis to include $\ell = 4$ modes is straightforward.

The objective is to compare the GW signal to physics at the horizon, which requires not only evaluating the perturbations at spatial infinity but also near the horizon. This introduces the first challenge: the precise location of the horizon. We started with two BHs, so the location or even the existence of a single horizon is non-trivial. Earlier CLA calculations suggest the formation of an apparent horizon that envelops both BHs [5]. We need to identify the parameters for which this apparent horizon forms and its location. Once determined, we can use the apparent horizon as "the" horizon and study its evolution over time. This may reveal nonlinear interactions at the horizon that imprint distinct features on the GW signal.

Once it is firmly established that the CLA is a viable approach for describing the merger phase, we can explore generalizations. The head-on collision with small initial momentum is not representative of most real-life astronomical events. Most BH collisions occur at ultra relativistic speeds, suggesting that the assumption of P being of the same order as L should be relaxed. This adjustment will result in higher ℓ-multipoles starting to contribute. Additionally, it would also be beneficial to look at generalising the system to a quasicircular inspiral rather than a head-on collision. This scenario is more astronomically accurate and emits significantly more energy as GWs [49, 50]. Such a system could still be treated with Bowen York initial data, but would involve another configuration for the extrinsic curvature.

Finally, the CLA could be adapted to a Kerr background instead of a Schwarzschild background for greater astrophysical accuracy. Within the CLA, this is relatively uncharted territory. While some work on second-order perturbation theory for Kerr has been conducted, it is primarily in the context of the self-force approach for extreme mass ratio inspirals (EMRIs), where one BH is significantly smaller than the other, and the mass ratio serves as the expansion parameter [51, 52]. This differs from the CLA, which considers BHs of the same mass. Several adaptations are required to modify the CLA to a Kerr background. First of all, an alternative type of initial data is needed, since the Bowen-York initial data does not represent a constant time slice of the Kerr spacetime [23, 35]. Furthermore, we have to evolve the perturbations using the Teukolsky equation [53], making it more appropriate to use a tetrad formulation [54, 55] instead of the coordinate-driven approach used here. A basis of spin-weighted harmonics, rather than tensorial harmonics, should also be employed (see e.g., [56]). Additionally, there is no equivalent of Eqs. (4.93)–(4.95) for Kerr, making it non-trivial to recover the metric perturbations from the master function described by the Teukolksy equation. This issue, known as metric reconstruction, will also have to be addressed in a second order framework [52, 57]. In summary, utilising a Kerr background introduces a unique set of challenges that require extensive research.

A Appendix: Gauge Transformations

GR is by nature a covariant theory, meaning that the physics it predicts does not depend on the chosen set of coordinates. This comprises the gauge freedom of GR. In terms of differential geometry, this freedom is the invariance of physics under the redefinition of the underlying manifold and its fields, such as the metric, by diffeomorphisms.

In this appendix we discuss the matter of gauge freedom in the context of perturbation theory. This discussion is based on [58], which offers a concise overview, and [45, 59], which provides a more complete, rigorous mathematical framework. First, we deliberate about gauge choices as identifications between the perturbed manifolds and background manifold. Then, we proceed to derive how quantities such as a vector and the metric change under second order gauge transformations.

A.1 Gauge Transformations in Perturbation Theory

In the context of perturbation theory, instead of working with a single manifold, we work with an infinite family of manifolds $\mathcal{M}_\epsilon$. The background, in particular, is denoted by $\mathcal{M}_0$. This family of spacetimes is parametrised by the expansion parameter ϵ. Each manifold $\mathcal{M}_\epsilon$ is equipped with a metric $g_{\mu\nu}(x;\epsilon)$. A choice of gauge in this setting corresponds to a choice of identification map ${\phi_\epsilon}^X : \mathcal{M}_0 \to \mathcal{M}_\epsilon$, which allows us to relate quantities on the perturbed manifold $\mathcal{M}_\epsilon$ to quantities on the background $\mathcal{M}_0$ via the pullback ${\phi_\epsilon}^{X*}$.[9] The flow of this identification map is generated by the vector field $X \equiv \frac{d{\phi_\epsilon}^X}{d\epsilon}$.

Making a gauge choice is equivalent to choosing a specific generator. We could as well have chosen some alternative generator Y with corresponding identification map ${\phi_\epsilon}^Y : \mathcal{M}_0 \to \mathcal{M}_\epsilon$. Switching from the identification as generated by X to the one generated by Y now corresponds to performing a gauge transformation. We have two equivalent ways of considering such a transformation: the *active* and *passive* viewpoint.

Suppose some point $p \in \mathcal{M}_0$ is mapped to some $q \in \mathcal{M}_\epsilon$ under the identification ${\phi_\epsilon}^X$ and to $q' \in \mathcal{M}_\epsilon$ under ${\phi_\epsilon}^Y$ (see Fig. 12). Now the map $\psi_\epsilon \equiv {\phi_\epsilon}^Y \circ ({\phi_\epsilon}^X)^{-1}$ constitutes a diffeomorphism on $\mathcal{M}_\epsilon$ such that $q' = \psi_\epsilon(q)$. Let T be some arbitrary tensor on $\mathcal{M}_\epsilon$ describing a physical quantity and let $\tilde{T} = \psi_\epsilon^* T$ be its pullback. Any physical predictions made by $(\mathcal{M}_\epsilon, T)$ are equally true for $(\mathcal{M}_\epsilon, \tilde{T})$, even though the diffeomorphism ψ_ϵ moved the points around [60]. This comprises the *active* interpretation, where a gauge transformation moves points.

Now suppose we have some coordinates x^μ on the base manifold $\mathcal{M}_0$, then the maps ${\phi_\epsilon}^X$ and ${\phi_\epsilon}^Y$ induce coordinates on the perturbed manifold $\mathcal{M}_\epsilon$ via their pullback. We shall treat X as the original gauge choice and let Y be an alternative gauge choice to which we would like to transform. In this fashion, we keep the label x^μ for the coordinates on $\mathcal{M}_\epsilon$ in gauge X, such that the point $q = {\phi_\epsilon}^X(p)$ has label $x^\mu(q) \equiv x^\mu(p)$. We can define an alternative coordinate system $y^\mu \equiv x^\mu \circ \psi_\epsilon^{-1}$, which satisfies the property $x^\mu(q) = y^\mu(q')$ (see Fig. 12). We may now treat the diffeomorphism ψ_ϵ as leaving p and all tensors at p unaltered, but inducing some coordinate change $x^\mu \to y^\mu$. This is the *passive* interpretation where gauge transformations leave points unchanged but change the chart.

We will now look further into expansions of these maps. To find the ϵ-expansion of this transformation, we consider the differing coordinate values of the points q and q' in $\mathcal{M}_\epsilon$. A general tensor T can be described on

[9] Smooth maps $\phi : \mathcal{M} \to \mathcal{N}$ have a natural way of pulling back functions and covariant tensor fields at $\Phi(p) \in \mathcal{N}$ to respective functions and fields at $p \in \mathcal{M}$. This is known as the *pullback* Φ^*. For its definition see [60, 61].

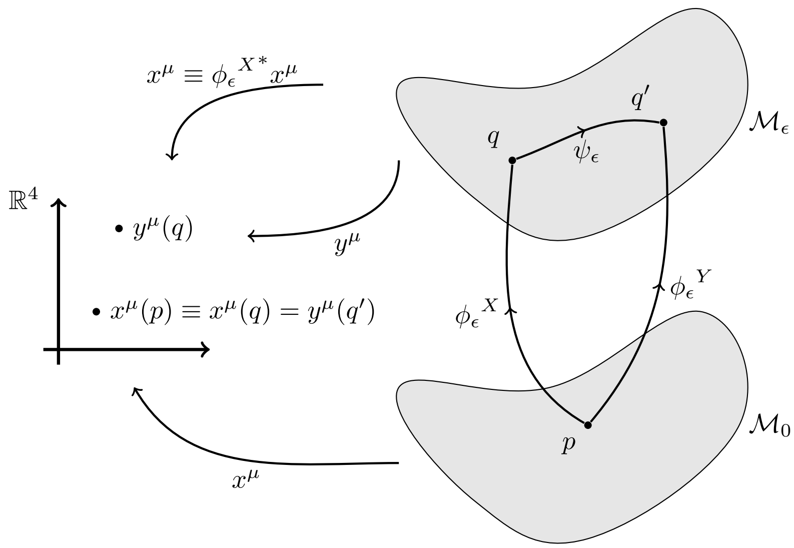


Figure 12: A gauge transformation corresponds to switching from one identification ${\phi_\epsilon}^X$ to another ${\phi_\epsilon}^Y$. The active viewpoint, where points are moved around, is shown on the right and the passive viewpoint, which is a change of chart, is represented on the left.

$\mathcal{M}_\epsilon$ by the Taylor approximation of its pullback via ${\phi_\epsilon}^Y$. As proven in [45], this approximation is given by

$$({\phi_\epsilon}^{Y*}T)(p) = (e^{\mathcal{L}_Y}T)(p) = \sum_{n=0}^{\infty} \frac{\epsilon^n}{n!}(\mathcal{L}_Y^n T)(p). \tag{A.1}$$

Before we apply Eq. (A.1) to the coordinate functions x^μ, we introduce the first and second order terms for the gauge transformation's generator ξ as follows[10]

$$^{(1)}\xi \equiv Y - X, \qquad ^{(2)}\xi \equiv \frac{1}{2}[X, Y]. \tag{A.2}$$

Applying Eq. (A.1) to each of the four coordinate functions x^μ for a given index μ, we obtain

$$\begin{aligned}
x^\mu(q') =& ({\phi_\epsilon}^{Y*}x^\mu)(p) \\
=& \sum_{n=0}^{\infty} \frac{\epsilon^n}{n!}(\mathcal{L}_Y^n x^\mu)(p) \\
=& x^\mu(p) + \epsilon(\mathcal{L}_Y x^\mu)(p) + \frac{1}{2}\epsilon^2(\mathcal{L}_Y^2 x^\mu)(p) + \mathcal{O}(\epsilon^3) \\
=& x^\mu(p) + \epsilon(\mathcal{L}_Y x^\mu - \mathcal{L}_X x^\mu)(p) \\
&+ \frac{1}{2}\epsilon^2(\mathcal{L}_X\mathcal{L}_Y x^\mu - \mathcal{L}_Y\mathcal{L}_X x^\mu + \mathcal{L}_Y^2 x^\mu - \mathcal{L}_Y\mathcal{L}_X x^\mu - \mathcal{L}_X\mathcal{L}_Y x^\mu + \mathcal{L}_X^2 x^\mu)(p) + \mathcal{O}(\epsilon^3) \\
=& x^\mu(q) + \epsilon(\mathcal{L}_{^{(1)}\xi} x^\mu)(p) + \epsilon^2\left[(\mathcal{L}_{^{(2)}\xi} x^\mu)(p) + \frac{1}{2}(\mathcal{L}_{^{(1)}\xi}^2 x^\mu)(p)\right] + \mathcal{O}(\epsilon^3) \\
=& x^\mu(q) + \epsilon\, {}^{(1)}\xi^\mu(x(q)) + \epsilon^2\left[{}^{(2)}\xi^\mu(x(q)) + \frac{1}{2}{}^{(1)}\xi^\nu(x(q))\partial_\nu {}^{(1)}\xi^\mu(x(q))\right] + \mathcal{O}(\epsilon^3).
\end{aligned} \tag{A.3}$$

[10]The reason why we make this particular choice of generator ξ can be found in Proposition 3 of [45].

where we repeatedly used that $\mathcal{L}_X x^\mu = 0$ throughout the calculation and used that $x^\mu(p) = x^\mu(q)$. Now think of a gauge transformation as a coordinate transformation $x^\mu \to y^\mu$. For small ϵ, this is a near-identity transformation. Per construction the new chart satisfies $y^\mu(q') = x^\mu(q)$. Rewriting Eq. (A.3) as an equation for $y^\mu(q')$, we find the coordinate transformation

$$\begin{aligned} y^\mu(q') &= x^\mu(q') - \epsilon\, {}^{(1)}\xi^\mu(x(q)) - \epsilon^2 \left[{}^{(2)}\xi^\mu(x(q)) + \frac{1}{2}\, {}^{(1)}\xi^\nu(x(q))\partial_\nu\, {}^{(1)}\xi^\mu(x(q)) \right] \\ &= x^\mu(q') - \epsilon\, {}^{(1)}\xi^\mu(x(q')) - \epsilon^2 \left[{}^{(2)}\xi^\mu(x(q')) - \frac{1}{2}\, {}^{(1)}\xi^\nu(x(q'))\partial_\nu\, {}^{(1)}\xi^\mu(x(q')) \right]. \end{aligned} \tag{A.4}$$

The key point here is that in the final step we have re-evaluated the first and second generators in the point $x(q')$ instead of $x(q)$. This can be accomplished by performing a Taylor expansion around $x(q')$, where we use Eq. (A.3) to express the distance between $x(q')$ and $x(q)$ in powers of ϵ. This yields the following expansions up to relevant order

$$\begin{aligned} {}^{(1)}\xi^\mu(x(q)) &= {}^{(1)}\xi^\mu(x(q')) + (x^\nu(q) - x^\nu(q'))\partial_\nu\, {}^{(1)}\xi^\mu(x(q')) + \mathcal{O}(\epsilon^2) \\ &= {}^{(1)}\xi^\mu(x(q')) - \epsilon\, {}^{(1)}\xi^\nu\partial_\nu\, {}^{(1)}\xi^\mu(x(q')) + \mathcal{O}(\epsilon^2), \\ {}^{(2)}\xi^\mu(x(q)) &= {}^{(2)}\xi^\mu(x(q')) + \mathcal{O}(\epsilon). \end{aligned}$$

Note that Eq. (A.3) and Eq. (A.4) provide the expressions for the coordinate transformation in the active and passive perspective, respectively. Both sides of Eq. (A.3) are formulated in the same chart x^μ, yet at different points q and q' in $\mathcal{M}_\epsilon$, entailing the active viewpoint. On the other hand, Eq. (A.4) is formulated at the same point $q \in \mathcal{M}_\epsilon$, but one side is defined in the chart y^μ while the other is defined in x^μ. This comprises the passive perspective.

A.2 Transformation of a Vector

To study the behaviour of tensors under the infinitesimal transformation above, we start by looking at a simple example: a vector. Let V be some vector field on the perturbed manifold $\mathcal{M}_\epsilon$ and denote its components given in the coordinates x^μ by V^μ. Recall that the diffeomorphism ψ_ϵ satisfies $q' = \psi_\epsilon(q)$. Denote the pullback of V over ψ_ϵ by $\tilde{V} = \psi_\epsilon^* V$. Now, in a passive interpretation to gauge transformations, we introduce a new chart $y^\mu \equiv x^\mu \circ \psi_\epsilon^{-1}$ as we have done before. Denote the components of V in the new coordinates y^μ as V'^μ. The pullback $\tilde{V}^\mu$ is related to V^μ and V'^μ by the following relation [45]

$$\tilde{V}^\mu(x(q)) = V'^\mu(y(q')) \equiv \left.\frac{\partial y^\mu}{\partial x^\nu}\right|_{x(q')} V^\nu(x(q')). \tag{A.5}$$

Now we want to find a transformation law. Recall that the coordinates satisfy $y^\mu(q') = x^\mu(q) \equiv x$, which is just some point in $\mathbb{R}^4$. Hence, Eq. (A.5) can simply be written as $\tilde{V}^\mu(x) = V'^\mu(x)$. If we manage to expand the RHS of Eq. (A.5) in terms of $x(q) = x$ instead of $x(q')$, we have managed to expand $V'^\mu(x)$ in terms of $V^\mu(x)$ evaluated at the same point x. This is the desired transformation law.

To perform this expansion, we start from the passive change of coordinates Eq. (A.4)

$$y^\mu(q') = x^\mu(q') - \epsilon\, {}^{(1)}\xi^\mu(x(q')) - \epsilon^2 \left[{}^{(2)}\xi^\mu(x(q')) - \frac{1}{2}\, {}^{(1)}\xi^\nu(x(q'))\partial_\nu\, {}^{(1)}\xi^\mu(x(q')) \right] + \mathcal{O}(\epsilon^3),$$

and proceed by calculating the Jacobian which up to second order in ϵ is given by

$$\begin{aligned}\frac{\partial y^\mu}{\partial x^\nu}\bigg|_{x(q')} =&\delta^\mu_\nu(x(q')) \\ &-\epsilon\partial_\nu{}^{(1)}\xi^\mu(x(q')) \\ &-\epsilon^2\left[\partial_\nu{}^{(2)}\xi^\mu(x(q'))-\frac{1}{2}\partial_\nu{}^{(1)}\xi^\lambda(x(q'))\partial_\lambda{}^{(1)}\xi^\mu(x(q'))-\frac{1}{2}{}^{(1)}\xi^\lambda(x(q'))\partial_\nu\partial_\lambda{}^{(1)}\xi^\mu(x(q'))\right]+\mathcal{O}(\epsilon^3).\end{aligned} \tag{A.6}$$

Now we insert this back into Eq. (A.5) to find the following expression

$$\begin{aligned}\tilde{V}^\mu(x(q)) =&\Bigg(\delta^\mu_\nu(x(q'))-\epsilon\partial_\nu{}^{(1)}\xi^\mu(x(q'))-\epsilon^2\Big[\partial_\nu{}^{(2)}\xi^\mu(x(q')) \\ &-\frac{1}{2}\partial_\nu{}^{(1)}\xi^\lambda(x(q'))\partial_\lambda{}^{(1)}\xi^\mu(x(q'))-\frac{1}{2}{}^{(1)}\xi^\lambda(x(q'))\partial_\nu\partial_\lambda{}^{(1)}\xi^\mu(x(q'))\Big]\Bigg)V^\nu(x(q'))+\mathcal{O}(\epsilon^3) \\ =&V^\mu(x(q')) \\ &-\epsilon\partial_\nu{}^{(1)}\xi^\mu(x(q'))V^\nu(x(q')) \\ &-\epsilon^2\left[\partial_\nu{}^{(2)}\xi^\mu(x(q'))-\frac{1}{2}\partial_\nu{}^{(1)}\xi^\lambda(x(q'))\partial_\lambda{}^{(1)}\xi^\mu(x(q'))-\frac{1}{2}{}^{(1)}\xi^\lambda(x(q'))\partial_\nu\partial_\lambda{}^{(1)}\xi^\mu(x(q'))\right]V^\nu(x(q'))+\mathcal{O}(\epsilon^3).\end{aligned}$$

We want to evaluate both sides of this equality at the point $x\in\mathbb{R}^4$. To this end, we expand all the terms on the RHS in terms of $x(q)=x$. For the term $\partial_\nu{}^{(1)}\xi^\mu(x(q'))$, one obtains

$$\partial_\nu{}^{(1)}\xi^\mu(x(q'))=\partial_\nu{}^{(1)}\xi^\mu(x(q))+\epsilon^{(1)}\xi^\alpha(x(q))\partial_\alpha\partial_\nu{}^{(1)}\xi^\mu(x(q))+\mathcal{O}(\epsilon^2), \tag{A.7}$$

and the expansion of the vector V^μ itself in terms of ϵ is given by

$$\begin{aligned}V^\nu(x(q')) =&V^\nu(x(q))+\left(\epsilon^{(1)}\xi^\alpha(x(q))+\epsilon^2\left[{}^{(2)}\xi^\alpha(x(q))+\frac{1}{2}{}^{(1)}\xi^\beta(x(q))\partial_\beta{}^{(1)}\xi^\alpha(x(q))\right]\right)\partial_\alpha V^\nu(x(q)) \\ &+\frac{1}{2}\epsilon^{2\,(1)}\xi^\alpha(x(q))^{(1)}\xi^\beta(x(q))\partial_\alpha\partial_\beta V^\nu(x(q))+\mathcal{O}(\epsilon^3).\end{aligned} \tag{A.8}$$

By inserting Eqs. (A.7)–(A.8) back into our expression $\tilde{V}^\mu(x(q))$ and carefully accounting for each ϵ, we find

$$\begin{aligned}
\tilde{V}^\mu(x(q)) =& V^\mu(x(q)) \\
&+ \epsilon\, {}^{(1)}\xi^\alpha x(q)\partial_\alpha V^\mu(x(q)) \\
&+ \epsilon^2 \left[{}^{(2)}\xi^\alpha x(q)\partial_\alpha + \frac{1}{2}{}^{(1)}\xi^\beta(x(q))\partial_\beta {}^{(1)}\xi^\alpha(x(q))\partial_\alpha + \frac{1}{2}{}^{(1)}\xi^\alpha(x(q)){}^{(1)}\xi^\beta(x(q))\partial_\alpha\partial_\beta \right] V^\mu(x(q)) \\
&- \epsilon\partial_\nu {}^{(1)}\xi^\mu(x(q)) \left(V^\nu(x(q)) + \epsilon\, {}^{(1)}\xi^\alpha(x(q))\partial_\alpha V^\nu(x(q)) \right) \\
&- \epsilon^2\, {}^{(1)}\xi^\alpha(x(q))\partial_\alpha\partial_\nu {}^{(1)}\xi^\mu(x(q))V^\nu(x(q)) \\
&- \epsilon^2 \partial_\nu {}^{(2)}\xi^\mu(x(q))V^\nu(x(q)) \\
&+ \frac{1}{2}\epsilon^2\partial_\nu {}^{(1)}\xi^\lambda(x(q))\partial_\lambda {}^{(1)}\xi^\mu(x(q))V^\nu(x(q)) \\
&+ \frac{1}{2}\epsilon^2\, {}^{(1)}\xi^\lambda(x(q))\partial_\nu\partial_\lambda {}^{(1)}\xi^\mu(x(q))V^\nu(x(q)) + \mathcal{O}(\epsilon^3) \\
=& V^\mu(x(q)) \\
&+ \epsilon \left[{}^{(1)}\xi^\alpha x(q)\partial_\alpha V^\mu(x(q)) - \partial_\alpha {}^{(1)}\xi^\mu(x(q))V^\alpha(x(q)) \right] \\
&+ \epsilon^2 \left[{}^{(2)}\xi^\alpha x(q)\partial_\alpha V^\mu(x(q)) - \partial_\alpha {}^{(2)}\xi^\mu(x(q))V^\alpha(x(q)) \right] \\
&+ \frac{1}{2}\epsilon^2 \Big[{}^{(1)}\xi^\beta(x(q))\partial_\beta {}^{(1)}\xi^\alpha(x(q))\partial_\alpha V^\mu(x(q)) + {}^{(1)}\xi^\alpha(x(q)){}^{(1)}\xi^\beta(x(q))\partial_\alpha\partial_\beta V^\mu(x(q)) \\
&- 2\partial_\nu {}^{(1)}\xi^\mu(x(q)){}^{(1)}\xi^\alpha(x(q))\partial_\alpha V^\nu(x(q)) + {}^{(1)}\xi^\alpha(x(q))\partial_\alpha\partial_\beta {}^{(1)}\xi^\mu(x(q))V^\beta(x(q)) \\
&+ \partial_\alpha {}^{(1)}\xi^\beta(x(q))\partial_\beta {}^{(1)}\xi^\mu(x(q))V^\alpha(x(q)) \Big] + \mathcal{O}(\epsilon^3).
\end{aligned}$$

When everything is sorted order by order, we can recognise different Lie-derivatives. We also use the first equality in Eq. (A.5) and identify $x(q) = x$ again to write the pullback in terms of $V'^\mu(x)$. This leads to the final expression for the gauge transformation

$$V'^\mu(x) = V^\mu(x) + \epsilon\mathcal{L}_{{}^{(1)}\xi}V^\mu(x) + \epsilon^2\left[\mathcal{L}_{{}^{(2)}\xi}V^\mu(x) + \frac{1}{2}\mathcal{L}^2_{{}^{(1)}\xi}V^\mu(x)\right] + \mathcal{O}(\epsilon^3). \tag{A.9}$$

A.3 Transformation of a metric

A similar story applies to the derivation for the metric's transformation. The derivation only involves an extra step, since it is covariant instead of contravariant and the algebra is far more messy since we are dealing with a rank-2 tensor field. The equivalent of Eq. (A.5) for the metric is

$$\tilde{g}_{\mu\nu}(x(q)) = g'_{\mu\nu}(y(q')) \equiv \left.\frac{\partial x^\lambda}{\partial y^\mu}\right|_{x(q')} \left.\frac{\partial x^\sigma}{\partial y^\nu}\right|_{x(q')} g_{\lambda\sigma}(x(q')). \tag{A.10}$$

Here, we stumble on the first problem as a consequence of the metric's covariance: the Jacobian $\partial x^\mu/\partial y^\nu|_{x(q')}$ is hard to calculate from Eq. (A.3), since it involves derivatives in other coordinates y^μ. Its inverse $\partial y^\mu/\partial x^\nu|_{x(q')}$, on the contrary, follows quite naturally as we have seen before. Using that the two matrices are each others inverse, i.e. $(\partial y^\mu/\partial x^\lambda)(\partial x^\lambda/\partial y^\nu) = \delta^\mu_\nu$, we have the equation

$$\begin{aligned}
\left(\delta^\mu_\lambda - \epsilon\partial_\lambda {}^{(1)}\xi^\mu - \epsilon^2\left[\partial_\lambda {}^{(2)}\xi^\mu - \frac{1}{2}\partial_\lambda {}^{(1)}\xi^\kappa\partial_\kappa {}^{(1)}\xi^\mu - \frac{1}{2}{}^{(1)}\xi^\kappa\partial_\lambda\partial_\kappa {}^{(1)}\xi^\mu\right] + \mathcal{O}(\epsilon^3)\right)\times \\
\left(A^\lambda_\nu + \epsilon B^\lambda_\nu + \epsilon^2 C^\lambda_\nu + \mathcal{O}(\epsilon^3)\right) = \delta^\mu_\nu,
\end{aligned}$$

where we dropped the coordinate labels $x(q')$ for notational convenience. This hierarchy of equation can be solved equation by equation and yields the following solution

$$\begin{aligned}
A_\nu^\lambda &= \delta_\nu^\lambda, \\
B_\nu^\lambda &= \partial_\nu {}^{(1)}\xi^\lambda, \\
C_\nu^\lambda &= \partial_\kappa {}^{(1)}\xi^\lambda \partial_\nu {}^{(1)}\xi^\kappa + \left[\partial_\nu {}^{(2)}\xi^\lambda - \frac{1}{2}\partial_\nu {}^{(1)}\xi^\kappa \partial_\kappa {}^{(1)}\xi^\lambda - \frac{1}{2} {}^{(1)}\xi^\kappa \partial_\nu \partial_\kappa {}^{(1)}\xi^\lambda\right].
\end{aligned}$$

Hence, the Jacobian becomes

$$\begin{aligned}
\left.\frac{\partial x^\mu}{\partial y^\nu}\right|_{x(q')} =& \delta_\nu^\mu(x(q')) + \epsilon \partial_\nu {}^{(1)}\xi^\mu(x(q')) \\
&+ \epsilon^2 \left[\partial_\nu {}^{(2)}\xi^\mu(x(q')) + \frac{1}{2}\partial_\kappa {}^{(1)}\xi^\mu(x(q'))\partial_\nu {}^{(1)}\xi^\kappa(x(q')) - \frac{1}{2} {}^{(1)}\xi^\kappa(x(q'))\partial_\nu\partial_\kappa {}^{(1)}\xi^\mu(x(q'))\right] + \mathcal{O}(\epsilon^3).
\end{aligned}$$

First we substitute this expression into Eq. (A.10), to obtain

$$\begin{aligned}
\tilde{g}_{\mu\nu}(x(q)) =& \Bigg(\delta_\mu^\rho \delta_\nu^\sigma + \epsilon\left[\delta_\mu^\rho \partial_\nu {}^{(1)}\xi^\sigma + \partial_\mu {}^{(1)}\xi^\rho \delta_\nu^\sigma\right] \\
&+ \epsilon^2 \Bigg[\delta_\mu^\rho \left(\partial_\nu {}^{(2)}\xi^\sigma + \frac{1}{2}\partial_\nu {}^{(1)}\xi^\kappa \partial_\kappa {}^{(1)}\xi^\sigma - \frac{1}{2} {}^{(1)}\xi^\kappa \partial_\nu \partial_\kappa {}^{(1)}\xi^\sigma\right) \\
&+ \left(\partial_\mu {}^{(2)}\xi^\rho + \frac{1}{2}\partial_\mu {}^{(1)}\xi^\lambda \partial_\lambda {}^{(1)}\xi^\rho - \frac{1}{2} {}^{(1)}\xi^\lambda \partial_\mu \partial_\lambda {}^{(1)}\xi^\rho\right)\delta_\nu^\sigma + (\partial_\mu {}^{(1)}\xi^\rho)(\partial_\nu {}^{(1)}\xi^\sigma)\Bigg]\Bigg) g_{\rho\sigma}(x(q'))) + \mathcal{O}(\epsilon^3) \\
=& g_{\mu\nu}(x(q')) \\
&+ \epsilon(\partial_\nu {}^{(1)}\xi^\sigma) g_{\mu\sigma}(x(q')) + \epsilon(\partial_\mu {}^{(1)}\xi^\rho) g_{\rho\nu}(x(q')) \\
&+ \epsilon^2 \left[\partial_\nu {}^{(2)}\xi^\sigma + \frac{1}{2}\partial_\nu {}^{(1)}\xi^\kappa \partial_\kappa {}^{(1)}\xi^\sigma - \frac{1}{2} {}^{(1)}\xi^\kappa \partial_\nu \partial_\kappa {}^{(1)}\xi^\sigma\right] g_{\mu\sigma}(x(q')) \\
&+ \epsilon^2 \left[\partial_\mu {}^{(2)}\xi^\rho + \frac{1}{2}\partial_\mu {}^{(1)}\xi^\lambda \partial_\lambda {}^{(1)}\xi^\rho - \frac{1}{2} {}^{(1)}\xi^\lambda \partial_\mu \partial_\lambda {}^{(1)}\xi^\rho\right] g_{\rho\nu}(x(q')) \\
&+ \epsilon^2 (\partial_\mu {}^{(1)}\xi^\rho)(\partial_\nu {}^{(1)}\xi^\sigma) g_{\rho\sigma}(x(q')) + \mathcal{O}(\epsilon^3),
\end{aligned}$$

where all terms on the RHS are evaluated in the point $x(q')$. We want to expand everything in terms of $x(q)$ again. Expanding the metric around $x(q)$ gives

$$\begin{aligned}
g_{\mu\nu}(x(q')) =& g_{\mu\nu}(x(q)) + \left(\epsilon {}^{(1)}\xi^\alpha(x(q)) + \epsilon^2\left[{}^{(2)}\xi^\alpha(x(q)) + \frac{1}{2} {}^{(1)}\xi^\beta(x(q))\partial_\beta {}^{(1)}\xi^\alpha(x(q))\right]\right)\partial_\alpha g_{\mu\nu} \\
&+ \frac{1}{2} {}^{(1)}\xi^\alpha(x(q)) {}^{(1)}\xi^\beta(x(q))\partial_\alpha\partial_\beta g_{\mu\nu} + \mathcal{O}(\epsilon^3).
\end{aligned} \tag{A.11}$$

Substituting Eq. (A.7) and (A.11) into the expression for the pullback of the metric to evaluate everything on the RHS in $x(q)$ yields the expression

$$
\begin{aligned}
\tilde{g}_{\mu\nu} =& g_{\mu\nu} \\
&+ \epsilon\, {}^{(1)}\xi^{\alpha}\partial_{\alpha} g_{\mu\nu} \\
&+ \epsilon^2 \left[{}^{(2)}\xi^{\alpha}\partial_{\alpha} + \frac{1}{2}\,{}^{(1)}\xi^{\beta}(\partial_{\beta}\,{}^{(1)}\xi^{\alpha})\partial_{\alpha} + \frac{1}{2}\,{}^{(1)}\xi^{\alpha}\,{}^{(1)}\xi^{\beta}\partial_{\alpha}\partial_{\beta} \right] g_{\mu\nu} \\
&+ \epsilon(\partial_{\nu}\,{}^{(1)}\xi^{\sigma}) \left(g_{\mu\sigma} + \epsilon\,{}^{(1)}\xi^{\alpha}\partial_{\alpha} g_{\mu\sigma} \right) \\
&+ \epsilon(\partial_{\mu}\,{}^{(1)}\xi^{\rho}) \left(g_{\rho\nu} + \epsilon\,{}^{(1)}\xi^{\beta}\partial_{\beta} g_{\rho\nu} \right) \\
&+ \epsilon^{2}\,{}^{(1)}\xi^{\beta}(\partial_{\beta}\partial_{\nu}\,{}^{(1)}\xi^{\sigma}) g_{\mu\sigma} + \epsilon^{2}\,{}^{(1)}\xi^{\alpha}(\partial_{\alpha}\partial_{\mu}\,{}^{(1)}\xi^{\rho}) g_{\rho\nu} \\
&+ \epsilon^2 \left[\partial_{\nu}\,{}^{(2)}\xi^{\sigma} + \frac{1}{2}\partial_{\nu}\,{}^{(1)}\xi^{\kappa}\partial_{\kappa}\,{}^{(1)}\xi^{\sigma} - \frac{1}{2}\,{}^{(1)}\xi^{\kappa}\partial_{\nu}\partial_{\kappa}\,{}^{(1)}\xi^{\sigma} \right] g_{\mu\sigma} \\
&+ \epsilon^2 \left[\partial_{\mu}\,{}^{(2)}\xi^{\rho} + \frac{1}{2}\partial_{\mu}\,{}^{(1)}\xi^{\lambda}\partial_{\lambda}\,{}^{(1)}\xi^{\rho} - \frac{1}{2}\,{}^{(1)}\xi^{\lambda}\partial_{\mu}\partial_{\lambda}\,{}^{(1)}\xi^{\rho} \right] g_{\rho\nu} \\
&+ \epsilon^2 (\partial_{\mu}\,{}^{(1)}\xi^{\rho})(\partial_{\nu}\,{}^{(1)}\xi^{\sigma}) g_{\rho\sigma} + \mathcal{O}(\epsilon^3) \\
=& g_{\mu\nu} \\
&+ \epsilon \left[{}^{(1)}\xi^{\alpha}\partial_{\alpha} g_{\mu\nu} + (\partial_{\nu}\,{}^{(1)}\xi^{\sigma}) g_{\mu\sigma} + (\partial_{\mu}\,{}^{(1)}\xi^{\rho}) g_{\rho\nu} \right] \\
&+ \epsilon^2 \left[{}^{(2)}\xi^{\alpha}\partial_{\alpha} g_{\mu\nu} + (\partial_{\nu}\,{}^{(2)}\xi^{\sigma}) g_{\mu\sigma} + (\partial_{\mu}\,{}^{(2)}\xi^{\rho}) g_{\rho\nu} \right] \\
&+ \frac{1}{2}\epsilon^2 \Big[{}^{(1)}\xi^{\beta}(\partial_{\beta}\,{}^{(1)}\xi^{\alpha})\partial_{\alpha} g_{\mu\nu} + {}^{(1)}\xi^{\alpha}\,{}^{(1)}\xi^{\beta}\partial_{\alpha}\partial_{\beta} g_{\mu\nu} + 2\,{}^{(1)}\xi^{\alpha}(\partial_{\nu}\,{}^{(1)}\xi^{\sigma})\partial_{\alpha} g_{\mu\sigma} + 2\,{}^{(1)}\xi^{\beta}(\partial_{\mu}\,{}^{(1)}\xi^{\rho})\partial_{\beta} g_{\rho\nu} \\
&+ {}^{(1)}\xi^{\beta}(\partial_{\beta}\partial_{\nu}\,{}^{(1)}\xi^{\sigma}) g_{\mu\sigma} + {}^{(1)}\xi^{\alpha}(\partial_{\alpha}\partial_{\mu}\,{}^{(1)}\xi^{\rho}) g_{\rho\nu} + (\partial_{\nu}\,{}^{(1)}\xi^{\kappa})(\partial_{\kappa}\,{}^{(1)}\xi^{\sigma}) g_{\mu\sigma} + (\partial_{\mu}\,{}^{(1)}\xi^{\lambda})(\partial_{\lambda}\,{}^{(1)}\xi^{\rho}) g_{\rho\nu} \\
&+ 2(\partial_{\mu}\,{}^{(1)}\xi^{\rho})(\partial_{\nu}\,{}^{(1)}\xi^{\sigma}) g_{\rho\sigma} \Big] + \mathcal{O}(\epsilon^3).
\end{aligned}
$$

Here, we recognise the same combinations of Lie derivatives as we have seen before in Eq. (A.9) after sorting everything order by order. This leads to the following transformation

$$g'_{\mu\nu}(x) = g_{\mu\nu}(x) + \epsilon \mathcal{L}_{{}^{(1)}\xi} g_{\mu\nu}(x) + \epsilon^2 \left[\mathcal{L}_{{}^{(2)}\xi} g_{\mu\nu}(x) + \frac{1}{2}\mathcal{L}^2_{{}^{(1)}\xi} g_{\mu\nu}(x) \right] + \mathcal{O}(\epsilon^3). \tag{A.12}$$

To get a complete order by order picture of the metric's gauge transformation, we also need to account for the fact that the metric itself has to be expanded as

$$g_{\mu\nu} = {}^{(0)}g_{\mu\nu} + \epsilon\, {}^{(1)}g_{\mu\nu} + \epsilon^2\, {}^{(2)}g_{\mu\nu} + \mathcal{O}(\epsilon^3). \tag{A.13}$$

This leads to the final expression

$$
\begin{aligned}
{}^{(0)}g'_{\mu\nu}(x) &= {}^{(0)}g_{\mu\nu}(x), \\
{}^{(1)}g'_{\mu\nu}(x) &= {}^{(1)}g_{\mu\nu}(x) + \mathcal{L}_{{}^{(1)}\xi}\, {}^{(0)}g_{\mu\nu}(x), \\
{}^{(2)}g'_{\mu\nu}(x) &= {}^{(2)}g_{\mu\nu}(x) + \mathcal{L}_{{}^{(2)}\xi}\, {}^{(0)}g_{\mu\nu}(x) + \mathcal{L}_{{}^{(1)}\xi}\, {}^{(1)}g_{\mu\nu}(x) + \frac{1}{2}\mathcal{L}^2_{{}^{(1)}\xi}\, {}^{(0)}g_{\mu\nu}(x).
\end{aligned}
$$

B Appendix: Expansion of the Einstein Equations

In order to derive the first and second order vacuum Einstein equations, we start by splitting up a generic metric $g_{\mu\nu}$ that can be expressed as some background metric $\bar{g}_{\mu\nu}$ plus some perturbations $h_{\mu\nu}$. This looks like

$$g_{\mu\nu} = \bar{g}_{\mu\nu} + \eta h_{\mu\nu}, \tag{B.1}$$

where η is the order parameter. Since we are interested in the vacuum Einstein equations $R_{\mu\nu} = 0$, we would like to determine the functional Taylor expansion

$$R_{\mu\nu}[\bar{g} + h] = \bar{R}_{\mu\nu}[\bar{g}] + \eta\, \delta R_{\mu\nu}[h] + \eta^2\, \delta^2 R_{\mu\nu}[h] + \mathcal{O}(\eta^3), \tag{B.2}$$

where the functional derivatives $\delta^n R_{\mu\nu}[h]$ are given by

$$\delta^n R_{\mu\nu}[\eta] \equiv \frac{1}{n!}\frac{d^n}{d\eta^n} R_{\mu\nu}[\bar{g} + \eta\phi]\bigg|_{\eta=0}, \tag{B.3}$$

for any rank-2 tensor $\phi_{\mu\nu}$. A similar definition applies to other tensors, which depend on the metric. The corrections $\delta R_{\mu\nu}[h]$ and $\delta^2 R_{\mu\nu}[h]$ can be derived by subsequently expanding the Christoffel symbols $\Gamma^\lambda{}_{\mu\nu}$ and the Riemann tensor $R^\rho{}_{\sigma\mu\nu}$. Taking a contraction with the metric finally yields the Ricci tensor.

First of all, we note that the inverse metric $g^{\mu\nu}$ can be expanded in h as

$$g^{\mu\nu} = \bar{g}^{\mu\nu} - \eta h^{\mu\nu} + \eta^2 h^\mu{}_\sigma h^{\sigma\nu} + \mathcal{O}(\eta^3). \tag{B.4}$$

This can be derived from the property that $g^{\mu\alpha} g_{\alpha\nu} = \delta^\mu{}_\nu$. By expanding this identity as

$$\delta^\mu{}_\nu = g^{\mu\alpha} g_{\alpha\nu} = \left(A^{\mu\alpha} + \eta B^{\mu\alpha} + \eta^2 C^{\mu\alpha}\right)\left(\bar{g}_{\alpha\nu} + \eta h_{\alpha\nu}\right),$$

we obtain a system of equations

$$\begin{aligned}
\delta^\mu{}_\nu &= A^{\mu\alpha}\bar{g}_{\alpha\nu}, \\
0 &= \left(A^{\mu\alpha} h_{\alpha\nu} + B^{\mu\alpha}\bar{g}_{\alpha\nu}\right), \\
0 &= \left(B^{\mu\alpha} h_{\alpha\nu} + C^{\mu\alpha}\bar{g}_{\alpha\nu}\right),
\end{aligned}$$

which can be solved step by step as $A^{\mu\alpha} = \bar{g}^{\mu\alpha}$, $B^{\mu\alpha} = -h^{\mu\alpha}$ and, finally, $C^{\mu\alpha} = h^\mu{}_\sigma h^{\sigma\alpha}$. Here we used the background metric $\bar{g}$ to raise indices; a convention that will be used for the rest of the calculations in this section.

To find the expansion

$$\Gamma^\lambda{}_{\mu\nu}[\bar{g} + h] = \bar{\Gamma}^\lambda{}_{\mu\nu}[\bar{g}] + \eta\, \delta\Gamma^\lambda{}_{\mu\nu}[h] + \eta^2\, \delta^2\Gamma^\lambda{}_{\mu\nu}[h] + \mathcal{O}(\eta^3), \tag{B.5}$$

for the Christoffel symbols, we start from their definition

$$\Gamma^\lambda{}_{\mu\nu} = \frac{1}{2} g^{\lambda\rho}(\partial_\mu g_{\rho\nu} + \partial_\nu g_{\mu\rho} - \partial_\rho g_{\mu\nu}). \tag{B.6}$$

When we take the functional derivative, we need the take the product rule into account. This yields

$$
\begin{aligned}
\delta\Gamma^{\lambda}{}_{\mu\nu}[h] &= \frac{d}{d\eta}\Gamma^{\lambda}{}_{\mu\nu}[\bar{g}+\eta h]\Big|_{\eta=0} \\
&= \left[\frac{1}{2}g^{\lambda\rho}\frac{d}{d\eta}\left(\partial_\mu g_{\rho\nu}+\partial_\nu g_{\mu\rho}-\partial_\rho g_{\mu\nu}\right)+\frac{1}{2}\frac{dg^{\lambda\rho}}{d\eta}\left(\partial_\mu g_{\rho\nu}+\partial_\nu g_{\mu\rho}-\partial_\rho g_{\mu\nu}\right)\right]\Big|_{\eta=0} \\
&=\frac{1}{2}\bar{g}^{\lambda\rho}\left(\partial_\mu \delta g_{\rho\nu}+\partial_\nu \delta g_{\mu\rho}-\partial_\rho \delta g_{\mu\nu}\right)+\frac{1}{2}\delta g^{\lambda\rho}\left(\partial_\mu \bar{g}_{\rho\nu}+\partial_\nu \bar{g}_{\mu\rho}-\partial_\rho \bar{g}_{\mu\nu}\right) \\
&=\frac{1}{2}\bar{g}^{\lambda\rho}\left(\partial_\mu h_{\rho\nu}+\partial_\nu h_{\mu\rho}-\partial_\rho h_{\mu\nu}\right)-\frac{1}{2}h^{\lambda\rho}\left(\partial_\mu \bar{g}_{\rho\nu}+\partial_\nu \bar{g}_{\mu\rho}-\partial_\rho \bar{g}_{\mu\nu}\right) \\
&=\frac{1}{2}\bar{g}^{\lambda\rho}\big(\bar{\nabla}_\mu h_{\rho\nu}+\bar{\Gamma}^{\sigma}{}_{\rho\mu}h_{\sigma\nu}+\bar{\Gamma}^{\sigma}{}_{\nu\mu}h_{\rho\sigma}+\bar{\nabla}_\nu h_{\mu\rho}+\bar{\Gamma}^{\sigma}{}_{\mu\nu}h_{\sigma\rho}+\bar{\Gamma}^{\sigma}{}_{\rho\nu}h_{\mu\sigma} \\
&\quad -\bar{\nabla}_\rho h_{\mu\nu}-\bar{\Gamma}^{\sigma}{}_{\mu\rho}h_{\sigma\nu}-\bar{\Gamma}^{\sigma}{}_{\nu\rho}h_{\mu\sigma}\big) \\
&\quad -\frac{1}{2}h_{\alpha\beta}\bar{g}^{\lambda\alpha}\bar{g}^{\rho\beta}\left(\partial_\mu \bar{g}_{\rho\nu}+\partial_\nu \bar{g}_{\mu\rho}-\partial_\rho \bar{g}_{\mu\nu}\right) \\
&=\frac{1}{2}\bar{g}^{\lambda\rho}\left(\bar{\nabla}_\mu h_{\rho\nu}+\bar{\nabla}_\nu h_{\mu\rho}-\bar{\nabla}_\rho h_{\mu\nu}\right)+\bar{g}^{\lambda\rho}\bar{\Gamma}^{\sigma}{}_{\mu\nu}h_{\sigma\rho}-\bar{g}^{\lambda\alpha}\bar{\Gamma}^{\beta}{}_{\mu\nu}h_{\alpha\beta} \\
&=\frac{1}{2}\bar{g}^{\lambda\rho}\left(\bar{\nabla}_\mu h_{\rho\nu}+\bar{\nabla}_\nu h_{\mu\rho}-\bar{\nabla}_\rho h_{\mu\nu}\right),
\end{aligned}
$$

where we used that $\delta g^{\lambda\rho} = -h^{\lambda\rho}$ and eliminated the partial derivatives of h by rewriting the formula for the covariant derivative $\bar{\nabla}$ of h. To summarise, the correction to the Christoffel symbols, linear in the perturbations, is given by

$$\delta\Gamma^{\lambda}{}_{\mu\nu}[h] = \frac{1}{2}\left(\bar{\nabla}_\mu h^{\lambda}{}_{\nu}+\bar{\nabla}_\nu h_{\mu}{}^{\lambda}-\bar{\nabla}^{\lambda}h_{\mu\nu}\right). \tag{B.7}$$

To find the quadratic corrections, we apply a functional derivative again. This amounts to

$$
\begin{aligned}
\delta^2\Gamma^{\lambda}{}_{\mu\nu}[h] =&\frac{1}{2!}\frac{d}{d\eta}\left[\frac{1}{2}g^{\lambda\rho}\frac{d}{d\eta}\left(\partial_\mu g_{\rho\nu}+\partial_\nu g_{\mu\rho}-\partial_\rho g_{\mu\nu}\right)+\frac{1}{2}\frac{dg^{\lambda\rho}}{d\eta}\left(\partial_\mu g_{\rho\nu}+\partial_\nu g_{\mu\rho}-\partial_\rho g_{\mu\nu}\right)\right]\Big|_{\eta=0} \\
=&\frac{1}{2}\Big[\frac{1}{2}g^{\lambda\rho}\frac{d^2}{d\eta^2}\left(\partial_\mu g_{\rho\nu}+\partial_\nu g_{\mu\rho}-\partial_\rho g_{\mu\nu}\right)+\frac{1}{2}\frac{dg^{\lambda\rho}}{d\eta}\frac{d}{d\eta}\left(\partial_\mu g_{\rho\nu}+\partial_\nu g_{\mu\rho}-\partial_\rho g_{\mu\nu}\right) \\
&+\frac{1}{2}\frac{dg^{\lambda\rho}}{d\eta}\frac{d}{d\eta}\left(\partial_\mu g_{\rho\nu}+\partial_\nu g_{\mu\rho}-\partial_\rho g_{\mu\nu}\right)+\frac{1}{2}\frac{d^2g^{\lambda\rho}}{d\eta^2}\left(\partial_\mu g_{\rho\nu}+\partial_\nu g_{\mu\rho}-\partial_\rho g_{\mu\nu}\right)\Big]\Big|_{\eta=0} \\
=&\frac{1}{2}\delta g^{\lambda\rho}\left(\partial_\mu h_{\rho\nu}+\partial_\nu h_{\mu\rho}-\partial_\rho h_{\mu\nu}\right)+\frac{1}{2}\delta^2 g^{\lambda\rho}\left(\partial_\mu \bar{g}_{\rho\nu}+\partial_\nu \bar{g}_{\mu\rho}-\partial_\rho \bar{g}_{\mu\nu}\right) \\
=&-\frac{1}{2}h^{\lambda\rho}\left(\partial_\mu h_{\rho\nu}+\partial_\nu h_{\mu\rho}-\partial_\rho h_{\mu\nu}\right)+\frac{1}{2}h^{\lambda}{}_{\sigma}h^{\sigma\rho}\left(\partial_\mu \bar{g}_{\rho\nu}+\partial_\nu \bar{g}_{\mu\rho}-\partial_\rho \bar{g}_{\mu\nu}\right) \\
=&-\frac{1}{2}h^{\lambda}{}_{\sigma}\left(\bar{\nabla}_\mu h^{\sigma}{}_{\nu}+\bar{\nabla}_\nu h_{\mu}{}^{\sigma}-\bar{\nabla}^{\sigma}h_{\mu\nu}\right).
\end{aligned}
$$

In the last step, a similar cancellation occurred as in the derivation of $\delta\Gamma^{\lambda}{}_{\mu\nu}[h]$, after introducing covariant derivatives. We observe that the quadratic correction is related to the linear correction by

$$\delta^2\Gamma^{\lambda}{}_{\mu\nu}[h] = -h^{\lambda}{}_{\sigma}\delta\Gamma^{\sigma}{}_{\mu\nu}[h]. \tag{B.8}$$

Now we turn to the Riemann tensor, which we will expand as

$$R^{\rho}{}_{\sigma\mu\nu}[\bar{g}+h] = R^{\rho}{}_{\sigma\mu\nu}[\bar{g}]+\eta\,\delta R^{\rho}{}_{\sigma\mu\nu}[h]+\eta^2\,\delta^2 R^{\rho}{}_{\sigma\mu\nu}[h]+\mathcal{O}(\eta^3). \tag{B.9}$$

From its definition as

$$R^{\rho}{}_{\sigma\mu\nu} = \partial_\mu\Gamma^{\rho}{}_{\nu\sigma}-\partial_\nu\Gamma^{\rho}{}_{\mu\sigma}+\Gamma^{\rho}{}_{\mu\lambda}\Gamma^{\lambda}{}_{\nu\sigma}-\Gamma^{\rho}{}_{\nu\lambda}\Gamma^{\lambda}{}_{\mu\sigma}, \tag{B.10}$$

it follows that its first functional derivative is given by

$$
\begin{aligned}
\delta R^{\rho}{}_{\sigma\mu\nu}[h] &= \frac{d}{d\eta} R^{\rho}{}_{\sigma\mu\nu}[\bar{g} + \eta h]\bigg|_{\eta=0} \\
&= \frac{d}{d\eta}\left[\partial_\mu \Gamma^{\rho}{}_{\nu\sigma} - \partial_\nu \Gamma^{\rho}{}_{\mu\sigma} + \Gamma^{\rho}{}_{\mu\lambda}\Gamma^{\lambda}{}_{\nu\sigma} - \Gamma^{\rho}{}_{\nu\lambda}\Gamma^{\lambda}{}_{\mu\sigma}\right]\bigg|_{\eta=0} \\
&= \left[\partial_\mu \frac{d}{d\eta}\Gamma^{\rho}{}_{\nu\sigma} - \partial_\nu \frac{d}{d\eta}\Gamma^{\rho}{}_{\mu\sigma} + \frac{d\Gamma^{\rho}{}_{\mu\lambda}}{d\eta}\Gamma^{\lambda}{}_{\nu\sigma} + \Gamma^{\rho}{}_{\mu\lambda}\frac{d\Gamma^{\lambda}{}_{\nu\sigma}}{d\eta} - \frac{d\Gamma^{\rho}{}_{\nu\lambda}}{d\eta}\Gamma^{\lambda}{}_{\mu\sigma} - \Gamma^{\rho}{}_{\nu\lambda}\frac{d\Gamma^{\lambda}{}_{\mu\sigma}}{d\eta}\right]\Bigg|_{\eta=0} \\
&= \partial_\mu \delta\Gamma^{\rho}{}_{\nu\sigma} - \partial_\nu \delta\Gamma^{\rho}{}_{\mu\sigma} + \delta\Gamma^{\rho}{}_{\mu\lambda}\bar{\Gamma}^{\lambda}{}_{\nu\sigma} + \bar{\Gamma}^{\rho}{}_{\mu\lambda}\delta\Gamma^{\lambda}{}_{\nu\sigma} - \delta\Gamma^{\rho}{}_{\nu\lambda}\bar{\Gamma}^{\lambda}{}_{\mu\sigma} - \bar{\Gamma}^{\rho}{}_{\nu\lambda}\delta\Gamma^{\lambda}{}_{\mu\sigma}.
\end{aligned}
$$

Here, we recognise the following two covariant derivatives

$$
\begin{aligned}
\bar{\nabla}_\mu \delta\Gamma^{\rho}{}_{\nu\sigma} &= \partial_\mu \delta\Gamma^{\rho}{}_{\nu\sigma} + \bar{\Gamma}^{\rho}{}_{\lambda\mu}\delta\Gamma^{\lambda}{}_{\nu\sigma} - \bar{\Gamma}^{\lambda}{}_{\nu\mu}\delta\Gamma^{\rho}{}_{\lambda\sigma} - \bar{\Gamma}^{\lambda}{}_{\sigma\mu}\delta\Gamma^{\rho}{}_{\nu\lambda}, \\
\bar{\nabla}_\nu \delta\Gamma^{\rho}{}_{\mu\sigma} &= \partial_\nu \delta\Gamma^{\rho}{}_{\mu\sigma} + \bar{\Gamma}^{\rho}{}_{\lambda\nu}\delta\Gamma^{\lambda}{}_{\mu\sigma} - \bar{\Gamma}^{\lambda}{}_{\mu\nu}\delta\Gamma^{\rho}{}_{\lambda\sigma} - \bar{\Gamma}^{\lambda}{}_{\sigma\nu}\delta\Gamma^{\rho}{}_{\mu\lambda},
\end{aligned}
$$

so that we obtain

$$
\delta R^{\rho}{}_{\sigma\mu\nu}[h] = \bar{\nabla}_\mu \delta\Gamma^{\rho}{}_{\nu\sigma} - \bar{\nabla}_\nu \delta\Gamma^{\rho}{}_{\mu\sigma}. \tag{B.11}
$$

We take another functional derivative to obtain the quadratic correction to the Riemann tensor:

$$
\begin{aligned}
\delta^2 R^{\rho}{}_{\sigma\mu\nu}[h] =& \frac{1}{2!}\frac{d}{d\eta}\left[\partial_\mu \frac{d}{d\eta}\Gamma^{\rho}{}_{\nu\sigma} - \partial_\nu \frac{d}{d\eta}\Gamma^{\rho}{}_{\mu\sigma} + \frac{d\Gamma^{\rho}{}_{\mu\lambda}}{d\eta}\Gamma^{\lambda}{}_{\nu\sigma} + \Gamma^{\rho}{}_{\mu\lambda}\frac{d\Gamma^{\lambda}{}_{\nu\sigma}}{d\eta} - \frac{d\Gamma^{\rho}{}_{\nu\lambda}}{d\eta}\Gamma^{\lambda}{}_{\mu\sigma} - \Gamma^{\rho}{}_{\nu\lambda}\frac{d\Gamma^{\lambda}{}_{\mu\sigma}}{d\eta}\right]\Bigg|_{\eta=0} \\
=& \frac{1}{2}\Bigg[\partial_\mu \frac{d^2}{d\eta^2}\Gamma^{\rho}{}_{\nu\sigma} - \partial_\nu \frac{d^2}{d\eta^2}\Gamma^{\rho}{}_{\mu\sigma} + \frac{d^2\Gamma^{\rho}{}_{\mu\lambda}}{d\eta^2}\Gamma^{\lambda}{}_{\nu\sigma} + \frac{d\Gamma^{\rho}{}_{\mu\lambda}}{d\eta}\frac{d\Gamma^{\lambda}{}_{\nu\sigma}}{d\eta} + \frac{d\Gamma^{\rho}{}_{\mu\lambda}}{d\eta}\frac{d\Gamma^{\lambda}{}_{\nu\sigma}}{d\eta} + \Gamma^{\rho}{}_{\mu\lambda}\frac{d^2\Gamma^{\lambda}{}_{\nu\sigma}}{d\eta^2} \\
&- \frac{d^2\Gamma^{\rho}{}_{\nu\lambda}}{d\eta^2}\Gamma^{\lambda}{}_{\mu\sigma} - \frac{d\Gamma^{\rho}{}_{\nu\lambda}}{d\eta}\frac{d\Gamma^{\lambda}{}_{\mu\sigma}}{d\eta} - \frac{d\Gamma^{\rho}{}_{\nu\lambda}}{d\eta}\frac{d\Gamma^{\lambda}{}_{\mu\sigma}}{d\eta} - \Gamma^{\rho}{}_{\nu\lambda}\frac{d^2\Gamma^{\lambda}{}_{\mu\sigma}}{d\eta^2}\Bigg]\Bigg|_{\eta=0} \\
=& \partial_\mu \delta^2\Gamma^{\rho}{}_{\nu\sigma} - \partial_\nu \delta^2\Gamma^{\rho}{}_{\mu\sigma} + \delta^2\Gamma^{\rho}{}_{\nu\lambda}\bar{\Gamma}^{\lambda}{}_{\mu\sigma} + \delta\Gamma^{\rho}{}_{\mu\lambda}\delta\Gamma^{\lambda}{}_{\nu\sigma} + \bar{\Gamma}^{\rho}{}_{\mu\lambda}\delta^2\Gamma^{\lambda}{}_{\nu\sigma} \\
&- \delta^2\Gamma^{\rho}{}_{\nu\lambda}\bar{\Gamma}^{\lambda}{}_{\mu\sigma} - \delta\Gamma^{\rho}{}_{\nu\lambda}\delta\Gamma^{\lambda}{}_{\mu\sigma} - \bar{\Gamma}^{\rho}{}_{\nu\lambda}\delta^2\Gamma^{\lambda}{}_{\mu\sigma}.
\end{aligned}
$$

Note that particular care has to be taken to account for the factor 1/2 in the definition of the functional derivatives. Again we recognise the covariant derivatives of the Christoffel symbol's first functional derivative. With this simplification, the second functional derivative becomes

$$
\delta^2 R^{\rho}{}_{\sigma\mu\nu}[h] = \bar{\nabla}_\mu \delta^2\Gamma^{\rho}{}_{\nu\sigma} - \bar{\nabla}_\nu \delta^2\Gamma^{\rho}{}_{\mu\sigma} + \delta\Gamma^{\rho}{}_{\mu\lambda}\delta\Gamma^{\lambda}{}_{\nu\sigma} - \delta\Gamma^{\rho}{}_{\nu\lambda}\delta\Gamma^{\lambda}{}_{\mu\sigma}. \tag{B.12}
$$

The Ricci tensor $R_{\mu\nu} = R^{\sigma}{}_{\mu\sigma\nu}$ can be calculated by performing a contraction. We find

$$
\delta R_{\mu\nu}[h] = \bar{\nabla}_\sigma \delta\Gamma^{\sigma}{}_{\nu\mu} - \bar{\nabla}_\nu \delta\Gamma^{\sigma}{}_{\sigma\mu}, \tag{B.13}
$$

$$
\delta^2 R_{\mu\nu}[h] = \bar{\nabla}_\sigma \delta^2\Gamma^{\sigma}{}_{\nu\mu} - \bar{\nabla}_\nu \delta^2\Gamma^{\sigma}{}_{\sigma\mu} + \delta\Gamma^{\sigma}{}_{\sigma\lambda}\delta\Gamma^{\lambda}{}_{\nu\mu} - \delta\Gamma^{\sigma}{}_{\nu\lambda}\delta\Gamma^{\lambda}{}_{\sigma\mu}. \tag{B.14}
$$

In terms of the metric perturbations $h_{\mu\nu}$ this becomes

$$\begin{aligned}
\delta R_{\mu\nu}[h] =& \frac{1}{2}\left(\bar{\nabla}_\sigma\bar{\nabla}_\nu h^\sigma{}_\mu + \bar{\nabla}_\sigma\bar{\nabla}_\mu h_\nu{}^\sigma - \bar{\nabla}_\sigma\bar{\nabla}^\sigma h_{\nu\mu}\right) \\
&- \frac{1}{2}\left(\bar{\nabla}_\nu\bar{\nabla}_\sigma h^\sigma{}_\mu + \bar{\nabla}_\nu\bar{\nabla}_\mu h_\sigma{}^\sigma - \bar{\nabla}_\nu\bar{\nabla}_\sigma h_{\sigma\mu}\right) \\
=& \frac{1}{2}\left(-\bar{\Box} h_{\mu\nu} - \bar{\nabla}_\nu\bar{\nabla}_\mu h + \bar{\nabla}_\sigma\bar{\nabla}_\nu h^\sigma{}_\mu + \bar{\nabla}_\sigma\bar{\nabla}_\mu h_\nu{}^\sigma\right), \\
\delta^2 R_{\mu\nu}[h] =& -\left(\bar{\nabla}_\sigma h^\sigma{}_\lambda\right)\delta\Gamma^\lambda{}_{\nu\mu} - h^\sigma{}_\lambda\bar{\nabla}_\sigma\delta\Gamma^\lambda{}_{\nu\mu} + \left(\bar{\nabla}_\nu h^\sigma{}_\lambda\right)\delta\Gamma^\lambda{}_{\sigma\mu} + h^\sigma{}_\lambda\bar{\nabla}_\nu\delta\Gamma^\lambda{}_{\sigma\mu} \\
&+ \frac{1}{4}\left(\bar{\nabla}_\sigma h^\sigma{}_\lambda + \bar{\nabla}_\lambda h_\sigma{}^\sigma - \bar{\nabla}^\sigma h_{\sigma\lambda}\right)\left(\bar{\nabla}_\nu h^\lambda{}_\mu + \bar{\nabla}_\mu h_\nu{}^\lambda - \bar{\nabla}^\lambda h_{\nu\mu}\right) \\
&- \frac{1}{4}\left(\bar{\nabla}_\nu h^\sigma{}_\lambda + \bar{\nabla}_\lambda h_\nu{}^\sigma - \bar{\nabla}^\sigma h_{\nu\lambda}\right)\left(\bar{\nabla}_\sigma h^\lambda{}_\mu + \bar{\nabla}_\mu h_\sigma{}^\lambda - \bar{\nabla}^\lambda h_{\sigma\mu}\right) \\
=& \frac{1}{2}h^{\sigma\lambda}\left(\bar{\nabla}_\nu\bar{\nabla}_\mu h_{\sigma\lambda} + \bar{\nabla}_\sigma\bar{\nabla}_\lambda h_{\nu\mu} - \bar{\nabla}_\sigma\bar{\nabla}_\nu h_{\lambda\mu} - \bar{\nabla}_\sigma\bar{\nabla}_\mu h_{\lambda\nu}\right) \\
&- \frac{1}{2}\left(\bar{\nabla}_\sigma h^\sigma{}_\lambda - \frac{1}{2}\bar{\nabla}_\lambda h\right)\left(\bar{\nabla}_\nu h^\lambda{}_\mu + \bar{\nabla}_\mu h_\nu{}^\lambda - \bar{\nabla}^\lambda h_{\nu\mu}\right) \\
&+ \frac{1}{4}\bar{\nabla}_\nu h^{\sigma\lambda}\bar{\nabla}_\mu h_{\sigma\lambda} + \frac{1}{2}\bar{\nabla}^\sigma h_\nu{}^\lambda\left(\bar{\nabla}_\sigma h_{\lambda\mu} - \bar{\nabla}_\lambda h_{\sigma\mu}\right),
\end{aligned}$$

where $\bar{\Box} \equiv \bar{g}^{\mu\nu}\bar{\nabla}_\mu\bar{\nabla}_\nu$ and the trace is defined by $h \equiv \bar{g}^{\mu\nu}h_{\mu\nu}$. These expressions agree with Eqs. (35.58) in [37]. Now we expand the metric perturbations up to second order:

$$h_{\mu\nu} = \epsilon\ {}^{(1)}g_{\mu\nu} + \epsilon^2\ {}^{(2)}g_{\mu\nu} + \mathcal{O}(\epsilon^3).$$

In terms of these perturbations the functional derivatives become

$$\begin{aligned}
\delta R_{\mu\nu}[h] =& \frac{1}{2}\epsilon\left(-\bar{\Box}\ {}^{(1)}g_{\mu\nu} - \bar{\nabla}_\nu\bar{\nabla}_\mu\ {}^{(1)}g + \bar{\nabla}_\sigma\bar{\nabla}_\nu\ {}^{(1)}g^\sigma{}_\mu + \bar{\nabla}_\sigma\bar{\nabla}_\mu\ {}^{(1)}g_\nu{}^\sigma\right) \\
&+ \frac{1}{2}\epsilon^2\left(-\bar{\Box}\ {}^{(2)}g_{\mu\nu} - \bar{\nabla}_\nu\bar{\nabla}_\mu\ {}^{(2)}g + \bar{\nabla}_\sigma\bar{\nabla}_\nu\ {}^{(2)}g^\sigma{}_\mu + \bar{\nabla}_\sigma\bar{\nabla}_\mu\ {}^{(2)}g_\nu{}^\sigma\right) + \mathcal{O}(\epsilon^3),
\end{aligned} \tag{B.15}$$

$$\begin{aligned}
\delta^2 R_{\mu\nu}[h] =& \frac{1}{2}\epsilon^2\Big[\ {}^{(1)}g^{\sigma\lambda}\left(\bar{\nabla}_\nu\bar{\nabla}_\mu\ {}^{(1)}g_{\sigma\lambda} + \bar{\nabla}_\sigma\bar{\nabla}_\lambda\ {}^{(1)}g_{\nu\mu} - \bar{\nabla}_\sigma\bar{\nabla}_\nu\ {}^{(1)}g_{\lambda\mu} - \bar{\nabla}_\sigma\bar{\nabla}_\mu\ {}^{(1)}g_{\lambda\nu}\right) \\
&- \left(\bar{\nabla}_\sigma\ {}^{(1)}g^\sigma{}_\lambda - \frac{1}{2}\bar{\nabla}_\lambda\ {}^{(1)}g\right)\left(\bar{\nabla}_\nu\ {}^{(1)}g^\lambda{}_\mu + \bar{\nabla}_\mu\ {}^{(1)}g_\nu{}^\lambda - \bar{\nabla}^\lambda\ {}^{(1)}g_{\nu\mu}\right) \\
&+ \frac{1}{2}\bar{\nabla}_\nu\ {}^{(1)}g_{\sigma\lambda}\bar{\nabla}_\mu\ {}^{(1)}g^{\sigma\lambda} + \bar{\nabla}^\sigma\ {}^{(1)}g_\nu{}^\lambda\left(\bar{\nabla}_\sigma\ {}^{(1)}g_{\lambda\mu} - \bar{\nabla}_\lambda\ {}^{(1)}g_{\sigma\mu}\right)\Big] + \mathcal{O}(\epsilon^3).
\end{aligned} \tag{B.16}$$

Ordering the terms in order of epsilon, we find the first and second vacuum Einstein equations

$${}^{(1)}R_{\mu\nu} = \delta R_{\mu\nu}[{}^{(1)}g] = 0, \tag{B.17}$$

$${}^{(2)}R_{\mu\nu} = \delta R_{\mu\nu}[{}^{(2)}g] + \delta^2 R_{\mu\nu}[{}^{(1)}g, {}^{(1)}g] = 0. \tag{B.18}$$

Hence, we obtain a hierarchy of equations. We can solve our system of equations by first solving the linearised Einstein equations (B.17) for ${}^{(1)}g$. Then, we substitute this solution in equation (B.18) to obtain a similar equation for ${}^{(2)}g$, but now with an addtional source term quadratic in ${}^{(1)}g$.

C Appendix: Spherical Decomposition

The Schwarzschild solution possesses a high degree of symmetry: it is both static and spherically symmetric. By virtue of these symmetries, all tensorial quantities on a Schwarzschild background can be split up into a separate spherical part and a (t, r)-part. In other words, the 4d spacetime $\mathcal{M}$ is factored as $\mathcal{M} = \mathcal{M}^2 \times \mathcal{S}^2$ where $\mathcal{S}^2$ is the 2d unit sphere and $\mathcal{M}^2$ represents the 2d (t, r)-subspace.

In this section, we will first introduce the necessary notation to be able to treat the quantities that are covariant on $\mathcal{M}^2$ or $\mathcal{S}^2$, separately. The notation and conventions in this appendix is largely based on [62] and [56]. Then, we continue by decomposing the quantities on the unit sphere in terms of spherical harmonics, which allows us to more easily treat problems multipole by multipole. We will decompose the metric in terms of ℓm modes, discuss how each multipole transforms under gauge transformations and decompose the vacuum Einstein equations.

We denote the coordinates on $\mathcal{M}^2$ as x^a and use the lowercase Latin alphabet $a, b, c, \ldots$ as the indices on its tangent bundle. Similarly, the coordinates for $\mathcal{S}^2$ are given by θ^A and we will use uppercase Latin indices $A, B, C, \ldots$ for its covariant quantities. For the full spacetime, we will use Greek indices $\alpha, \beta, \gamma, \ldots$. The metric in Schwarzschild coordinates $x^\mu = (t, r, \theta, \varphi)$ given by

$$ds^2 = g_{\mu\nu}\, dx^\mu dx^\nu = -\left(1 - \frac{2M}{r}\right) dt^2 + -\left(1 - \frac{2M}{r}\right)^{-1} dr^2 + r^2(d\theta^2 + \sin^2\theta d\varphi^2).$$

can now be expressed as a product metric of the metric g_{ab} on $\mathcal{M}^2$ and the round metric Ω_{AB} on $\mathcal{S}^2$, written as

$$ds^2 = g_{ab}\, dx^a dx^b + r^2 \Omega_{AB}\, d\theta^A d\theta^B. \tag{C.1}$$

In coordinates $x^a = (t, r)$ and $\theta^A = (\theta, \varphi)$, the submetrics take the form

$$g_{ab} = \operatorname{diag}\left(-\left(1 - \frac{2M}{r}\right), \left(1 - \frac{2M}{r}\right)^{-1}\right), \quad \Omega_{AB} = \operatorname{diag}(1, \sin^2\theta). \tag{C.2}$$

The covariant derivative on $\mathcal{M}^2$ compatible with the metric g_{ab} is denoted by $\mathcal{D}$ and the covariant derivative on $\mathcal{S}^2$ compatible with Ω_{AB} by D. The covariant derivative compatible with the full metric $g_{\mu\nu}$ is denoted as ∇ with Christoffel symbols $\Gamma^\lambda{}_{\mu\nu}$. For the Christoffel symbols corresponding to $\mathcal{D}$ and D, we have $\Gamma^c{}_{ab}[\mathcal{D}] \equiv \Gamma^c{}_{ab}$ and $\Gamma^C{}_{AB}[D] \equiv \Gamma^C{}_{AB}$, respectively. The only non-vanishing Christoffel symbols with mixed indices are

$$\begin{aligned}
\Gamma^a{}_{AB} &= \frac{1}{2} g^{a\lambda} \left(\partial_A g_{\lambda B} + \partial_B g_{A\lambda} - \partial_\lambda g_{AB}\right) \\
&= -\frac{1}{2} \partial^a g_{AB} \\
&= -r r^a \Omega_{AB}, \\
\Gamma^A{}_{Bc} &= \frac{1}{2} g^{A\lambda} \left(\partial_B g_{\lambda c} + \partial_c g_{B\lambda} - \partial_\lambda g_{Bc}\right) \\
&= \frac{1}{2} g^{AC} \partial_c g_{BC} \\
&= \frac{1}{r} r_c \delta^A{}_B,
\end{aligned}$$

where we introduced the notation $\partial_a r \equiv r_a$. The covariant derivative $\nabla_\mu V^\nu$ of a vector V, as a consequence, has the following possible projections of its indices on the submanifolds

$$\nabla_a V^b = \partial_a V^b + \Gamma^b{}_{\lambda a} V^\lambda = \partial_a V^b + \Gamma^b{}_{ca} V^c = \mathcal{D}_a V^b, \tag{C.3}$$
$$\nabla_a V^B = \partial_a V^B + \Gamma^B{}_{\lambda a} V^\lambda = \partial_a V^B + \Gamma^B{}_{Ca} V^C = \mathcal{D}_a V^B + r^{-1} r_a V^B, \tag{C.4}$$
$$\nabla_A V^b = \partial_A V^b + \Gamma^b{}_{\lambda A} V^\lambda = \partial_A V^b + \Gamma^b{}_{CA} V^C = D_A V^b - r r^b \Omega_{CA} V^C, \tag{C.5}$$
$$\nabla_A V^B = \partial_A V^B + \Gamma^B{}_{\lambda A} V^\lambda = \partial_A V^B + \Gamma^B{}_{CA} V^C + \Gamma^B{}_{cA} V^c = D_A V^B + r^{-1} r_c \delta_A{}^B V^c. \tag{C.6}$$

Note that in the last step in both Eq. (C.4) and (C.5), we replaced the partial derivatives by covariant derivatives. This is due to the fact that V^B lives in the vectorbundle of $\mathcal{S}^2$ and as consequence can be regarded as a scalar function on $\mathcal{M}^2$, in the case of Eq. (C.4), and vice versa for Eq. (C.5). Hence, we can replace the partial derivatives $\partial_a V^B$ and $\partial_A V^b$ by the covariant derivatives on $\mathcal{M}^2$ given by $\mathcal{D}_a V^B$ and on $\mathcal{S}^2$ given by $D_A V^b$, respectively. A covector ω_ν, similarly, satisfies

$$\nabla_a \omega_b = \mathcal{D}_a \omega_b, \tag{C.7}$$
$$\nabla_a \omega_B = \mathcal{D}_a \omega_B - r^{-1} r_a \omega_B, \tag{C.8}$$
$$\nabla_A \omega_b = D_A \omega_b - r^{-1} r_b \omega_A, \tag{C.9}$$
$$\nabla_A \omega_B = D_A \omega_B + r r^c \Omega_{AB} \omega_c. \tag{C.10}$$

These rules can easily be extended to tensors of higher rank by applying the corresponding rule index by index to each projected index.

We are interested in perturbations on this spherically symmetric background, in particular the metric perturbations. An arbitrary metric perturbation $h_{\mu\nu}$ can be decomposed in ℓm multipoles as[11]

$$h_{ab} = \sum_{\ell m} f_{ab}^{\ell m}(r,t)\, Y^{\ell m}, \tag{C.11}$$
$$h_{aB} = \sum_{\ell m} j_a^{\mathrm{even},\ell m}\, D_B Y^{\ell m} + j_a^{\mathrm{odd},\ell m}\, \epsilon_A{}^B D_B Y^{\ell m}, \tag{C.12}$$
$$h_{AB} = \sum_{\ell m} r^2 \left[K^{\ell m}(r,t)\, Y^{\ell m} \Omega_{AB} + G^{\ell m}(r,t) D_A D_B Y^{\ell m}\right] + h_2^{\mathrm{odd},\ell m}(r,t)\, \epsilon_{(A}{}^C D_{B)} D_C Y^{\ell m}, \tag{C.13}$$

where $\epsilon_A{}^B$ is the Levi-Civita tensor and where we grouped together the perturbations that have the same index structure in the following way

$$f_{ab}^{\ell m} = \begin{pmatrix} \left(1 - \frac{2M}{r}\right) H_0^{\ell m} & H_1^{\ell m} \\ H_1^{\ell m} & \left(1 - \frac{2M}{r}\right)^{-1} H_2^{\ell m} \end{pmatrix}, \quad j_a^{\mathrm{even},\ell m} = \begin{pmatrix} h_0^{\mathrm{even},\ell m} \\ h_1^{\mathrm{even},\ell m} \end{pmatrix}, \quad j_a^{\mathrm{odd},\ell m} = \begin{pmatrix} h_0^{\mathrm{odd},\ell m} \\ h_1^{\mathrm{odd},\ell m} \end{pmatrix}. \tag{C.14}$$

Here, we have a set of seven even parity perturbations $H_0, H_1, H_2, h_0^{\mathrm{even}}, h_1^{\mathrm{even}}, K, G$ whose harmonics do not change under reflections on the sphere and a set of three odd perturbations $h_0^{\mathrm{odd}}, h_1^{\mathrm{odd}}, h_2^{\mathrm{odd}}$ whose harmonics flip sign under a reflection. In this work, we are mainly interested in the even perturbations, but we will include the odd perturbations for completeness.

[11] To better correspond with the rest of this work, we opted to use $D_A D_B Y^{\ell m}$ in correspondence with [39, 40] instead of the more modern $Y_{AB}^{\ell m} \equiv \left[D_A D_B + \frac{1}{2}\ell(\ell+1)\Omega_{AB}\right] Y^{\ell m}$ in [62]. Hence, the definition of K here is slightly different. The relation to K_{martel} in [62] is $K = K_{\mathrm{martel}} + \ell(\ell+1)G$.

C.1 Regge-Wheeler Gauge

Due to the background's spherical symmetry, we can also factor out the spherical dependence for the gauge transformations. Recall that gauge transformations are generated by a vector ${}^{(i)}\xi_\mu$. This vector can be decomposed in tensorial harmonics as

$$\begin{aligned} {}^{(i)}\xi_a &= \sum_{\ell m} {}^{(i)}\mathcal{A}_a{}^{\ell m}(t,r)\, Y^{\ell m}, \\ {}^{(i)}\xi_A &= \sum_{\ell m} {}^{(i)}\mathcal{B}^{\ell m}(t,r)\, D_A Y^{\ell m} + {}^{(i)}\mathcal{C}^{\ell m}(t,r)\, \epsilon_A{}^B D_B Y^{\ell m}. \end{aligned} \tag{C.15}$$

Hence, we do not have to worry about the angular (θ,φ)-coordinates anymore and only have to account for the t and r dependence when specifying a suitable generator for our transformation. The even sector is governed by the coefficients ${}^{(i)}\mathcal{A}_a{}^{\ell m}(t,r)$ and ${}^{(i)}\mathcal{B}^{\ell m}(t,r)$ and the odd sector is governed by ${}^{(i)}\mathcal{C}^{\ell m}(t,r)$.

Recall that at first order a first order gauge transformation transforms the perturbations by

$$ {}^{(1)}g'_{\mu\nu} = {}^{(1)}g_{\mu\nu} + \mathcal{L}_{{}^{(1)}\xi}\, {}^{(0)}g_{\mu\nu}. $$

Therefore, the first order perturbations are amended by a term

$$ \Delta\, {}^{(1)}g_{\mu\nu} \equiv {}^{(1)}g'_{\mu\nu} - {}^{(1)}g_{\mu\nu} = 2\nabla_{(\mu}\, {}^{(1)}\xi_{\nu)}. $$

after the first order transformation. We apply the rules in Eqs. (C.7)–(C.8) to the covariant derivative and insert Eq. (C.15), in order to determine how each Regge-Wheeler perturbation changes exactly. Note that at first order all multipoles decouple and each lm mode is only influenced by ${}^{(1)}\xi_\mu{}^{\ell m}$. For the even perturbations, where we suppress the ℓm-label in the notation, the transformation laws yield

$$\begin{aligned} {}^{(1)}f'_{ab} &= {}^{(1)}f_{ab} + 2\mathcal{D}_{(a}\, {}^{(1)}\mathcal{A}_{b)}, \\ {}^{(1)}j'^{\text{even}}{}_a &= {}^{(1)}j^{\text{even}}{}_a + {}^{(1)}\mathcal{A}_a + \mathcal{D}_a\, {}^{(1)}\mathcal{B} - \frac{2}{r} r_a\, {}^{(1)}\mathcal{B}, \\ {}^{(1)}K' &= {}^{(1)}K + \frac{2}{r} r^a\, {}^{(1)}\mathcal{A}_a, \\ {}^{(1)}G' &= {}^{(1)}G + \frac{2}{r^2}\, {}^{(1)}\mathcal{B}. \end{aligned}$$

When we express the $\mathcal{D}$ covariant derivatives on $\mathcal{M}^2$ in (t, r)-coordinates and split out each component by Eq. (C.14), we find that the Regge-Wheeler quantities are changed by the terms

$$\Delta^{(1)}H_0 = \frac{2r}{r-2M}\partial_t{}^{(1)}\mathcal{A}_t - \frac{2M}{r^2}{}^{(1)}\mathcal{A}_r, \tag{C.16}$$

$$\Delta^{(1)}H_1 = \partial_t{}^{(1)}\mathcal{A}_r + \partial_r{}^{(1)}\mathcal{A}_t - \frac{2M}{r^2}\left(1-\frac{2M}{r}\right)^{-1}{}^{(1)}\mathcal{A}_t, \tag{C.17}$$

$$\Delta^{(1)}H_2 = \left(1-\frac{2M}{r}\right)\partial_r{}^{(1)}\mathcal{A}_r + \frac{2M}{r^2}{}^{(1)}\mathcal{A}_r, \tag{C.18}$$

$$\Delta^{(1)}h_0{}^{\text{even}} = {}^{(1)}\mathcal{A}_t + \partial_t{}^{(1)}\mathcal{B}, \tag{C.19}$$

$$\Delta^{(1)}h_1{}^{\text{even}} = {}^{(1)}\mathcal{A}_r + \partial_r{}^{(1)}\mathcal{B} - \frac{2}{r}{}^{(1)}\mathcal{B}, \tag{C.20}$$

$$\Delta^{(1)}K = \frac{2}{r}\left(1-\frac{2M}{r}\right){}^{(1)}\mathcal{A}_r, \tag{C.21}$$

$$\Delta^{(1)}G = \frac{2}{r^2}{}^{(1)}\mathcal{B}. \tag{C.22}$$

Observe that we can express the generator's coefficients as

$${}^{(1)}\mathcal{B} = \frac{r^2}{2}\Delta^{(1)}G, \quad {}^{(1)}\mathcal{A}_a = \Delta^{(1)}j^{\text{even}}{}_a - \frac{r^2}{2}\partial_a\Delta^{(1)}G. \tag{C.23}$$

As a consequence, we can formulate gauge invariant quantities based on f_{ab} and K by adding terms that will cancel Δf_{ab} and ΔK, respectively. These cancellation terms can be found by simply replacing ${}^{(1)}\mathcal{B} \to -\frac{r^2}{2}{}^{(1)}G$ and ${}^{(1)}\mathcal{A}_a \to -\left({}^{(1)}j^{\text{even}}{}_a - \frac{r^2}{2}\partial_a{}^{(1)}G\right)$ in Eqs. (C.16)–(C.18) and Eq. (C.21). This yields the following quantities, which are invariant under first order gauge transformations

$${}^{(1)}\tilde{H}_0 \equiv {}^{(1)}H_0 + \frac{2M}{r^2}{}^{(1)}h_1{}^{\text{even}} - M\partial_r{}^{(1)}G - \frac{2r}{r-2M}\partial_t{}^{(1)}h_0{}^{\text{even}} + \frac{r^3}{r-2M}\partial_t^2{}^{(1)}G, \tag{C.24}$$

$${}^{(1)}\tilde{H}_1 \equiv {}^{(1)}H_1 + \frac{2M}{r^2-2Mr}{}^{(1)}h_0{}^{\text{even}} - \partial_r{}^{(1)}h_0{}^{\text{even}} - \partial_t{}^{(1)}h_1{}^{\text{even}} + \frac{r(r-3M)}{r-2M}\partial_t{}^{(1)}G + r^2\partial_t\partial_r{}^{(1)}G, \tag{C.25}$$

$${}^{(1)}\tilde{H}_2 \equiv {}^{(1)}H_2 - \frac{2M}{r^2}{}^{(1)}h_1{}^{\text{even}} - \frac{2(r-2M)}{r}\partial_r{}^{(1)}h_1{}^{\text{even}} + (2r-3M)\partial_r{}^{(1)}G + r(r-2M)\partial_t^2{}^{(1)}G, \tag{C.26}$$

$${}^{(1)}\tilde{K} \equiv {}^{(1)}K - \frac{2}{r}\left(1-\frac{2M}{r}\right)\left[{}^{(1)}h_1{}^{\text{even}} - \frac{r^2}{2}\partial_r{}^{(1)}G\right]. \tag{C.27}$$

These invariant quantities motivate a particularly easy gauge choice: the Regge-Wheeler gauge. For even perturbations this choice amounts to setting $G = h_0^{\text{even}} = h_1^{\text{even}} = 0$. In this case, all cancellation terms in the gauge invariant quantities vanish. Hence, the metric perturbations in the Regge-Wheeler gauge simply correspond to the gauge invariant quantities. It is always possible to choose ${}^{(1)}\mathcal{A}_a$ and ${}^{(1)}\mathcal{B}$ in such a way, albeit locally, that the Regge-Wheeler gauge is attained.

For the odd perturbations a similar story applies. Although it is not essential to our calculations, which only concern even perturbations, we will include the odd transformations here for completeness. The projection of the covariant derivative of the generator for the odd perturbations yields

$$\begin{aligned}{}^{(1)}j'^{\text{odd}}{}_a &= {}^{(1)}j^{\text{odd}}{}_a + \mathcal{D}_a{}^{(1)}\mathcal{C} - \tfrac{2}{r}r_a{}^{(1)}\mathcal{C},\\ {}^{(1)}h_2'^{\text{ odd}} &= {}^{(1)}h_2{}^{\text{odd}} + 2{}^{(1)}\mathcal{C},\end{aligned}$$

where we again suppresed the ℓm-labels. For the odd perturbations, it is easy to see that ${}^{(1)}\mathcal{C} = \frac{1}{2}\Delta\,{}^{(1)}h_2{}^{\text{odd}}$. The odd gauge invariant quantities therefore are

$$\begin{aligned}{}^{(1)}\tilde{h}_0^{\text{odd}} &\equiv {}^{(1)}h_0{}^{\text{odd}} - \tfrac{1}{2}\partial_t\,{}^{(1)}h_2{}^{\text{odd}},\\ {}^{(1)}\tilde{h}_1^{\text{odd}} &\equiv {}^{(1)}h_1{}^{\text{odd}} - \tfrac{1}{2}\partial_r\,{}^{(1)}h_2{}^{\text{odd}} + \tfrac{1}{r}\,{}^{(1)}h_2{}^{\text{odd}}.\end{aligned}$$

The Regge-Wheeler gauge for the odd perturbations is now given by ${}^{(1)}h_2{}^{\text{odd}} = 0$ such that ${}^{(1)}\tilde{h}_0^{\text{odd}} = {}^{(1)}h_0{}^{\text{odd,RW}}$ and ${}^{(1)}\tilde{h}_1^{\text{odd}} = {}^{(1)}h_1{}^{\text{odd,RW}}$.

At second order, things get significantly more involved. The second order perturbations transform both as a consequence of the *pure* second order perturbation generated by ${}^{(2)}\xi_\mu$, as well the effects of the first order transformation ${}^{(1)}\xi_\mu$. The metric perturbations transform as

$${}^{(2)}g'_{\mu\nu} = {}^{(2)}g_{\mu\nu} + \mathcal{L}_{{}^{(2)}\xi}\,{}^{(0)}g_{\mu\nu} + \mathcal{L}_{{}^{(1)}\xi}\,{}^{(1)}g_{\mu\nu} + \frac{1}{2}\mathcal{L}^2_{{}^{(1)}\xi}\,{}^{(0)}g_{\mu\nu},$$

so after a gauge transformation we have to add the term

$$\begin{aligned}\Delta\,{}^{(2)}g_{\mu\nu} = {}& 2\nabla_{(\mu}{}^{(2)}\xi_{\nu)}\\ &+ {}^{(1)}\xi^\lambda\nabla_\alpha\,{}^{(1)}g_{\mu\nu} + 2\,{}^{(1)}g_{\lambda(\mu}\nabla_{\nu)}{}^{(1)}\xi^\lambda\\ &+ {}^{(1)}\xi^\lambda\nabla_\lambda\nabla_{(\mu}{}^{(1)}\xi_{\nu)} + \nabla_\lambda{}^{(1)}\xi_{(\mu}\nabla_{\nu)}{}^{(1)}\xi^\lambda + \nabla_\mu{}^{(1)}\xi^\lambda\nabla_\nu{}^{(1)}\xi^\alpha.\end{aligned}$$

The quadratic terms in the first order perturbations and generators cause mixing between the different ℓm multipoles. This makes it difficult to provide general expressions. In the remainder of this discussion we will restrict ourselves to the $(\ell = 2, m = 0)$ even perturbations.

The terms, with which we have to amend second order Regge-Wheeler quantities after a gauge transformation, are calculated in `M2xS2-Split_Coordinates_Final.nb` [43]. Most are too lengthy and impractical to present in print. The shortest term is given by

$$\begin{aligned}\Delta^{(2)}G = {}& \frac{2}{r^2}{}^{(2)}\mathcal{B} + \frac{1}{70r^5(r-2M)}\Bigg(96r^2(r-2M)^2\,{}^{(1)}h_1\,{}^{(1)}\mathcal{A}_r - 96r^4\,{}^{(1)}h_0\,{}^{(1)}\mathcal{A}_t - 236Mr^3\,{}^{(1)}K\,{}^{(1)}\mathcal{B}\\ &+ 118r^4\,{}^{(1)}K\,{}^{(1)}\mathcal{B} - 192M^2\,{}^{(1)}\mathcal{B}^2 + 1092Mr\,{}^{(1)}\mathcal{B}^2 - 498r^2\,{}^{(1)}\mathcal{B}^2\\ &- 2(r-2M)r^3\,{}^{(1)}G\big(59(2M-r)\,{}^{(1)}\mathcal{A}_r + 402\,{}^{(1)}\mathcal{B}(t,\ r)\big) + 236M^2r^4\,{}^{(1)}\mathcal{A}_r\,\frac{\partial\,{}^{(1)}G}{\partial r}\\ &- 236Mr^5\,{}^{(1)}\mathcal{A}_r\frac{\partial\,{}^{(1)}G(t,\ r)}{\partial r} + 59r^6\,{}^{(1)}\mathcal{A}_r\,\frac{\partial\,{}^{(1)}G}{\partial r} + 428M^2r^2\,{}^{(1)}\mathcal{A}_r\frac{\partial\,{}^{(1)}\mathcal{B}}{\partial r}\\ &- 428Mr^3\,{}^{(1)}\mathcal{A}_r\frac{\partial\,{}^{(1)}\mathcal{B}}{\partial r} + 107r^4\,{}^{(1)}\mathcal{A}_r\frac{\partial\,{}^{(1)}\mathcal{B}}{\partial r} - 59r^6\,{}^{(1)}\mathcal{A}_t\frac{\partial\,{}^{(1)}G(t,\ r)}{\partial t} - 107r^4\,{}^{(1)}\mathcal{A}_t\,\frac{\partial\,{}^{(1)}\mathcal{B}}{\partial t}\Bigg).\end{aligned}$$

In the literature, this term can also be found in Eq. (36) of [46]. Even when accounting for some convention differences, such as factors 1/2 in the gauge transformation and a factor r^2 in the definition of ${}^{(1)}K$ and ${}^{(1)}G$, the expressions do not agree.

At this point, gauge invariance can mean two things: invariance under *pure* second order transformations and invariance under *full* second order gauge transformation, including first order effects. The former is very easy to address. The quantities invariant under pure second order transformations are simply the first order ones as found in Eqs. (C.24)–(C.27) with (1) replaced by (2) everywhere. If one wants to set up quantities that are invariant under the full second order transformation, this requires more care due to the extra quadratic first order terms (see [46]). To define fully invariant quantities, quadratic terms need to constructed that under a first order transformation cancel the quadratic terms that arise as a consequence of the Lie derivatives at second order.

C.2 Vacuum Einstein Equations

The evolution of the perturbations is governed by the Einstein Equations, which we also have to decompose in their $\mathcal{S}^2$ and $\mathcal{M}^2$ parts. To this end, we decompose the corrections to the Ricci tensor $\delta R_{\mu\nu}$ and $\delta^2 R_{\mu\nu}$ in Eqs. (2.23)–(2.24). The calculations can be found in the Mathematica notebooks `M2xS2-Split_Final.nb` and `M2xS2-Split_Coordinates_Final.nb` [43]. In terms of some generic perturbation $h_{\mu\nu}$, the Ricci tensor $\delta R_{\mu\nu}$ exhibits the following projections

$$
\begin{aligned}
\delta R_{ab} =& \tfrac{1}{2}\mathcal{D}_c\left(\mathcal{D}_a h_b{}^c + \mathcal{D}_b h_a{}^c - \mathcal{D}^c h_{ab}\right) - \tfrac{1}{2}\mathcal{D}_b\mathcal{D}_a h^c{}_c + \frac{1}{r}r^c\left(\mathcal{D}_a h_{bc} + \mathcal{D}_b h_{ac} - \mathcal{D}_c h_{ab}\right)\\
&+ \frac{1}{2r^2}D^C\left(\mathcal{D}_a h_{bC} + \mathcal{D}_b h_{aC}\right) - \frac{1}{2r^2}\mathcal{D}_b\mathcal{D}_a h^C{}_C - \frac{1}{2r^2}D^C D_C h_{ab}\\
&+ \frac{1}{2r^3}\left(r_a\mathcal{D}_b h^C{}_C + r_b\mathcal{D}_a h^C{}_C\right) + \frac{1}{r^3}h^C{}_C\mathcal{D}_b r_a - \frac{1}{r^4}r_a r_b h^C{}_C,\\
\delta R_{aB} =& \tfrac{1}{2}\mathcal{D}^c\mathcal{D}_a h_{Bc} + \tfrac{1}{2}\mathcal{D}^c D_B h_{ac} - \tfrac{1}{2}D_B\mathcal{D}_a h^c{}_c - \tfrac{1}{2}\Box h_{aB}\\
&+ \frac{1}{2r}r_a D_B h^c{}_c + \frac{1}{r}r^c\mathcal{D}_a h_{Bc} - \frac{1}{r}h_B{}^c\mathcal{D}_c r_a - \frac{1}{r}r_a\mathcal{D}^c h_{Bc}\\
&+ \frac{1}{2r^2}D^C D_B h_{aC} - \frac{1}{2r^2}D^C D_C h_{aB} + \frac{1}{2r^2}D^C\mathcal{D}_a h_{BC} - \frac{1}{2r^2}D_B\mathcal{D}_a h^C{}_C - \frac{1}{r^2}r_a r^c h_{Bc}\\
&+ \frac{1}{r^3}r_a D_B h^C{}_C - \frac{1}{r^3}r_a D^C h_{BC},\\
\delta R_{AB} =& r r^a\mathcal{D}^b(h_{ab} - \frac{1}{2}g_{ab}h^c{}_c)\Omega_{AB} + (r^a r^b + r\mathcal{D}^a r^b)h_{ab}\Omega_{AB} - \tfrac{1}{2}D_B D_A h^c{}_c + \tfrac{1}{2}\mathcal{D}^c\left(D_A h_{Bc} + D_B h_{Ac}\right)\\
&- \tfrac{1}{2}\Box h_{AB} + \frac{1}{r}r^c\mathcal{D}_c(h_{AB} - \frac{1}{2}\Omega_{AB}h^C{}_C) + \frac{1}{r}\Omega_{AB}r^c D_C h_a{}^C + \frac{1}{2r^2}D_C\left(D_A h_B{}^C + D_B h_A{}^C - D^C h_{AB}\right)\\
&- \frac{2}{r^2}r^c r_c(h_{AB} - \frac{1}{2}h^C{}_C) - \frac{1}{2r^2}D_B D_A h^C{}_C.
\end{aligned}
$$

where $\Box = \mathcal{D}_c\mathcal{D}^c$ denotes the d'Alembertian on $\mathcal{M}^2$. These expressions agree with the expressions provided in the Appendix B of [62]. Now we specialise to the Regge-Wheeler perturbations, as provided in Eqs. (C.11)–(C.14). In our case, we are solely interested in the even perturbations. Furthermore, we impose the Regge-Wheeler gauge which will greatly simplify the matter, since we have $h^{\mathrm{RW}}_{aB} = 0$ for the mixed projections. This yields the expressions

$$\begin{aligned}\delta R_{ab}^{\mathrm{RW}} =&\Bigg[\frac{\ell(\ell+1)}{2r^2}f_{ab} + \frac{1}{2}\mathcal{D}_c\left(\mathcal{D}_a f_b{}^c + \mathcal{D}_b f_a{}^c - \mathcal{D}^c f_{ab}\right) - \frac{1}{2}\mathcal{D}_a\mathcal{D}_b f_c{}^c \\ &+ \frac{1}{r}r^c\left(\mathcal{D}_a f_{bc} + \mathcal{D}_b f_{ac} - \mathcal{D}_c f_{ab} - \frac{2}{r}r_{(a}\mathcal{D}_{b)}K - \mathcal{D}_a\mathcal{D}_b K\right)\Bigg]Y^{\ell m},\end{aligned} \tag{C.28}$$

$$\delta R_{aB}^{\mathrm{RW}} = \frac{1}{2}\left[\mathcal{D}^c f_{ac} - \mathcal{D}_a f^c{}_c + \frac{1}{r}r_a f^c{}_c - \mathcal{D}_a K\right] D_B Y^{\ell m}, \tag{C.29}$$

$$\begin{aligned}\delta R_{AB}^{\mathrm{RW}} =&\Bigg[r^a r^b f_{ab} + r\mathcal{D}^a r^b\, f_{ab} + r r^a \mathcal{D}^b f_{ab} - \frac{1}{2} r r^a \mathcal{D}_a f_c{}^c \\ &- \frac{1}{2}\Box(r^2 K) + \frac{1}{2}\ell(\ell+1)K - r_a r^a K - 2 r r^a \mathcal{D}_a K - K r \mathcal{D}_a r^a\Bigg]\Omega_{AB}Y^{\ell m} \\ &- \frac{1}{2} f_c{}^c D_A D_B Y^{\ell m},\end{aligned} \tag{C.30}$$

Note that in [62], they calculate the Einstein equation including mass-energy source terms. Hence, the Eqs. (4.13)–(4.16) there contain additional terms as a consequence of the linearised Ricci scalar δR.

The expressions for the quadratic Ricce tensor $\delta^2 R_{\mu\nu}$, are rather long and would not be illuminating to provide in print. For the projections of $\delta^2 R_{\mu\nu}$, in terms of a generic perturbation $h_{\mu\nu}$, we refer to `M2xS2-Split_Final.nb` [43]. The expressions given specifically in the RW gauge are

$$\begin{aligned}\delta^2 R_{ab}^{\mathrm{RW},(20)\times(20)} = \Big[& \tfrac{1}{4}\mathcal{D}_a f^{cd}\mathcal{D}_b f_{cd} + \tfrac{1}{4}(\mathcal{D}_a f_b{}^c + \mathcal{D}_b f_a{}^c - \mathcal{D}^c f_{ab})\mathcal{D}_c h^d{}_d \\ & - \tfrac{1}{2}(\mathcal{D}_a f_b{}^c + \mathcal{D}_b f_a{}^c - \mathcal{D}^c f_{ab})\mathcal{D}_d f_c{}^d + \tfrac{1}{2}(\mathcal{D}_d f_{bc} - \mathcal{D}_c f_{bd})\mathcal{D}^d f_a{}^c \\ & - \frac{1}{2} f^{cd}(\mathcal{D}_a\mathcal{D}_d f_{bc} + \mathcal{D}_b\mathcal{D}_d f_{ac} - \mathcal{D}_d\mathcal{D}_c f_{ab} - \mathcal{D}_a\mathcal{D}_b f_{cd}) \\ & - \frac{1}{r}K r^c(\mathcal{D}_a f_{bc} + \mathcal{D}_b f_{ac} - \mathcal{D}_c f_{ab}) - \frac{1}{r} r^c f_c{}^d(\mathcal{D}_a f_{bd} + \mathcal{D}_b f_{ad} - \mathcal{D}_d f_{ab}) \\ & - \frac{1}{r}K(f_a{}^c\mathcal{D}_c r_b + f_b{}^c\mathcal{D}_c r_a) - \frac{1}{2r^2}\ell(\ell+1)K f_{ab} \\ & + \frac{4}{r^2}K^2 r_a r_b + \frac{1}{r^2}K\mathcal{D}_a\mathcal{D}_b(r^2K) + \frac{1}{2r^2}(\mathcal{D}_a f_b{}^c + \mathcal{D}_b f_a{}^c - \mathcal{D}^c f_{ab})\mathcal{D}_c(r^2K) \\ & - \frac{2}{r^3}K(r_a\mathcal{D}_b(r^2K) + r_b\mathcal{D}_a(r^2K)) + \frac{1}{2r^4}\mathcal{D}_a(r^2K)\mathcal{D}_b(r^2K)\Big] Y^{20}Y^{20} \\ & + \frac{1}{2r^2}(f_{ac}f_b{}^c - \tfrac{1}{2}f_c{}^c f_{ab})D_A Y^{20} D^A Y^{20},\end{aligned} \tag{C.31}$$

$$\begin{aligned}\delta^2 R_{aB}^{\mathrm{RW},(20)\times(20)} = \Big[& \tfrac{1}{2} f^{bc}\mathcal{D}_a f_{bc} - \tfrac{1}{2}(\mathcal{D}_b f^{bc} - \tfrac{1}{2}\mathcal{D}_c f_b{}^b) f_{ac} + \tfrac{1}{4}\mathcal{D}_a f^{bc}\, f_{bc} - \tfrac{1}{2} f^{bc}\mathcal{D}_c f_{ab} \\ & - \frac{1}{2r} r_a(K f_c{}^c + f^{bc} f_{bc}) + \frac{1}{r^2}K\mathcal{D}_a(r^2K) + \frac{1}{4r^2}\mathcal{D}_a(r^2K) f_c{}^c\Big] Y^{20} D_B Y^{20},\end{aligned} \tag{C.32}$$

$$\begin{aligned}\delta^2 R_{AB}^{\mathrm{RW},(20)\times(20)} = \Big[& \frac{r}{2} r^a(f^{bc}\mathcal{D}_a f_{bc} + f_a{}^b\mathcal{D}_b f_c{}^c) - rK f^{ab}\mathcal{D}_a r_b - r r^a(f^{bc}\mathcal{D}_c f_{ab} + f_a{}^b\mathcal{D}_c f_b^c) \\ & - r^a r^b f_a{}^c f_{bc} - \tfrac{1}{4}\mathcal{D}_a f_b^b\mathcal{D}_a(r^2K) + \tfrac{1}{2}\mathcal{D}^a(r^2K)\mathcal{D}_b f_a{}^b + \tfrac{1}{2} f^{ab}\mathcal{D}_a\mathcal{D}_b(r^2K)\Big]\Omega_{AB} Y^{20}Y^{20} \\ & + \tfrac{1}{2} f^{ab} f_{ab} Y^{20} D_A D_B Y^{20} + \left[\tfrac{1}{4} f^{ab} f_{ab} + \tfrac{1}{2}K f_a{}^a\right] D_A Y^{20}\, D_B Y^{20} \\ & + \left[\tfrac{1}{2}K^2 - \tfrac{1}{4}K f_a{}^a\right]\Omega_{AB} D_C Y^{20}\, D^C Y^{20},\end{aligned} \tag{C.33}$$

where we suppressed the $\ell m = 20$ superscripts for $f_{ab}^{\ell m}$ and $K^{\ell m}$. In this case, where we only consider the $\ell = 2$ mode, the expression is still quite simple because we have the same mode contributing twice. When we consider different modes ℓm and $\ell' m'$, however, we also have to account for there being different $f_{ab}^{\ell m}$ and $f_{ab}^{\ell' m'}$ etc. which will somewhat complicate the expressions.

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