

Second order gauge invariant gravitational perturbations of a Kerr black hole

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We investigate higher than the first order gravitational perturbations in the Newman-Penrose formalism. Equations for the Weyl scalar ψ_4 , representing outgoing gravitational radiation, can be uncoupled into a single wave equation to any perturbative order. For second order perturbations about a Kerr black hole, we prove the existence of a first and second order gauge (coordinates) and tetrad invariant waveform, ψ_I , by explicit construction. This waveform is formed by the second order piece of ψ_4 plus a term, quadratic in first order perturbations, chosen to make ψ_I totally invariant and to have the appropriate behavior in an asymptotically flat gauge. ψ_I fulfills a single wave equation of the form $\mathcal{T}\psi_I = S$, where \mathcal{T} is the same wave operator as for first order perturbations and S is a source term build up out of (known to this level) first order perturbations. We discuss the issues of imposition of initial data to this equation, computation of the energy and momentum radiated and wave extraction for direct comparison with full numerical approaches to solve Einstein equations.

I. MOTIVATIONS AND OVERVIEW

The prediction of accurate waveforms generated during the final orbital stage of binary black holes has become a worldwide research topic in general relativity during this decade. The main reason is that these catastrophic astrophysical events, considered one of the strongest sources of gravitational radiation in the universe, are potentially observable by LIGO, VIRGO and other interferometric detectors. For its strong nonlinear features this black hole merger problem is only fully tractable by direct numerical integration (with supercomputers) of Einstein equations. Several difficulties remain to be solved in this approach such as the presence of early instabilities in the codes for numerical evolution of Einstein theory [1], and finding a new prescription for astrophysically realistic initial data representing orbiting black holes [2,3]. Meanwhile, perturbation theory has shown not only to be the main approximation scheme for computation of gravitational radiation, but also a useful tool to provide benchmarks for full numerical simulations. From the theoretical point of view perhaps the more relevant contribution during the nineties in perturbative theory has been the “close limit approximation” [4]. It considers the final merger state of two black holes as described by a *single* perturbed one. This idea was applied to the head-on collision of two black holes and the emitted gravitational radiation was computed by means of the techniques used in first order perturbation theory around a Schwarzschild black hole. When the results of this computation have been compared with those of the full numerical integration of Einstein equations the agreement was so good that it was disturbing [5]. This encouraged the significant effort invested into the development of a second order Zerilli formalism of metric perturbations about the Schwarzschild background. The method was successfully implemented with particular emphasis on the comparison with the fully numerically generated results. In the case of two initially stationary black holes (Misner data) the agreement of the results is striking [6]. Second order perturbation theory confirmed the success of the close limit approximation with an impressive agreement in both waveforms and energy radiated against the full numerical simulations. There has been a tantamount success in the extension of these studies to the case of initially moving towards each other black holes [7], and for slowly rotating ones [8] (See Ref. [9] for a comprehensive review).

All the above close limit computations are based on the Zerilli [10] approach to metric perturbations of a Schwarzschild, i.e. nonrotating, black hole. This method uses the Regge-Wheeler [11] decomposition of the metric perturbations into multipoles (tensor harmonics). Einstein equations in the Regge-Wheeler gauge reduce to two

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single wave equations for the even and odd parity modes of the gravitational perturbations. There is, however, the strong belief that binary black holes in a realistic astrophysical scenario merge together into a single, highly rotating, black hole. There is also concrete observational evidence of accreting black holes [12] that places the rotation parameter as high as $a/M \simeq 0.95$. Finally, highly rotating black holes provide a new scenario to compare perturbative theory with full numerical integrations of Einstein equations.

The Regge-Wheeler-Zerilli techniques cannot be extended to study perturbations on a Kerr black hole background (see Ref. [8] for the slowly rotating case). In this case there is not a multipole decomposition of metric perturbations (in the time domain) and Einstein equations cannot be uncoupled into wave equations. A reformulation of the gravitational field equations due to Newman and Penrose [13], based on the Einstein equations and Bianchi identities projected along a null tetrad, allowed Teukolsky [14] to write down a single master wave equation for the perturbations of the Kerr metric in terms of the Weyl scalars ψ_4 or ψ_0 . This formulation has several advantages: i) It is a first order gauge invariant description. ii) It does not rely on any frequency or multipole decomposition. iii) The Weyl scalars are objects defined in the full nonlinear theory and a one parameter perturbative expansion of it was proved to provide a reliable account of the problem [15]. In addition, the Newman-Penrose formulation constitutes a simpler and more elegant framework to organize higher order perturbation schemes as we will see in the next section.

Since the seventies the Teukolsky equation for the first order perturbations around a rotating black hole has been Fourier transformed and integrated in the frequency domain for a variety of situations where initial data played no role (see Ref. [16] for a review). Very recently it was proved [17,18] that nothing is intrinsically wrong with the Teukolsky equation when sources extend to infinity and that a regularization method produces sensible results. In order to incorporate initial data and have a notable computational efficiency, concrete progress has been made recently to complete a computational framework that allows to integrate the Teukolsky equation in the *time domain*: First, an evolution code for integration of the Teukolsky wave equation is now available [19] and successfully tested [20]. Second, non conformally flat Cauchy data, compatible with Boyer-Lindquist slices of the Kerr geometry, began to be studied with a Kerr-Schild [21,22] or an axially symmetric [23,24] ansatz. Finally, an expression connecting ψ_4 to only Cauchy data has been worked out explicitly [25,20,26].

Assuming that we can solve for the first order perturbations problem, we decided to go one step forward in setting the formalism for the second order perturbations. As motivations for this work we can cite the spectacular results presented in Ref. [6] for the head-on collision and the hope to obtain similar agreement for the orbital binary black hole case in the close limit. Second order perturbations of the Kerr metric may even play a more important role in this case since we expect the perturbative parameter to be linear in the separation of the holes [27] while in the head on case it is quadratic in the separation [29]. The nonrotating limit of our approach will also provide an independent test and clarify some aspects of Ref. [6] results. High precision comparison with full numerical integration of Einstein equations using perturbative theory as benchmarks is also one of the main goals in this program as well as a the development of a tool to explore a complementary region of the parameter space to that reachable by full numerical methods. An important application of second order perturbations is to provide error bars. It is well known that linearized perturbation theory does not provide, in itself, any indication on how good the perturbative approximation is. In fact, it is in general very difficult to estimate the errors involved in replacing an exact solution of the full Einstein equations with an approximate (perturbative) solution, i.e., to determine how small a perturbative parameter ε must be in order that the approximate solution have sufficient accuracy. Moreover, first order perturbation theory can be very sensitive to the choice of parametrization, i. e. different choices of the perturbative parameter can affect the accuracy of the linearized approximation [28]. The only reliable procedure to resolve the error and/or parameter arbitrariness is to carry out computations of the radiated waveforms and energy to second order in the expansion parameter. The ratio of second order corrections to the linear order results constitutes the only direct and systematically independent measure of the goodness of the perturbation results.

In the next section we extend to second (and higher) order the Teukolsky derivation of the equation that describes first order perturbations about a Kerr hole. To do so we consider the Newman-Penrose [13] formulation of the Bianchi identities and Einstein equations, make a perturbative expansion of it, and decouple the equation that describes the evolution of second (and higher) order perturbations. This equation takes the following form

$$\widehat{\mathcal{T}}\psi^{(2)} = S[\psi^{(1)}, \partial_t\psi^{(1)}], \quad (1)$$

where $\psi \doteq (\rho^{(0)})^{-4}\psi_4$, $\widehat{\mathcal{T}}$ is the same (zeroth order) wave operator that applies to first order perturbations (see Eq. (12)) and S is a source term quadratic in the first order perturbations (see Eqs. (9)-(11)).

In Section III.A we describe how to compute the source, appearing in Eq. (1), in terms of solutions of the wave equations for $\psi_4^{(1)}$ or $\psi_0^{(1)}$ only, which are the objects we directly obtain from the integration of the first order Teukolsky equation. Sec. III.B discusses the issue of building up $\psi_4^{(2)}$ and $\partial_t\psi_4^{(2)}$ out of initial data (that we assume are given to first and second order). In section III.C we recall the equations for the computation of the second order total radiated energy and momentum.

Higher than first order calculations are always characterized by an extraordinary complexity and a number of subtle, potentially confusing, gauge issues mainly due to the fact that a general second order gauge invariant formulation is not yet at hand in the literature. In general, gauge invariant quantities have an inherent physical meaning and they automatically lead to the simpler and direct interpretation of the results. In the Newman-Penrose formalism one has not only to look at gauge invariance (i. e. invariance under infinitesimal coordinate transformations), but also at invariance under tetrad rotations (see Sections IV.A and IV.B). More specifically, the problem here is that the waveform $\psi_4^{(2)}$ in Eq. (1) is neither first order coordinate gauge invariant nor tetrad invariant. The question that arises therefore is whether $\psi_4^{(2)}$ can be unambiguously compared with, for instance, full numerical computations of the covariant ψ_4^{Num} . To handle this problem we build up a coordinate and tetrad invariant quantity up to second order, $\psi_I^{(2)}$, which has the property of reducing to the linear part (in the second order perturbations of the metric) of $\psi_4^{(2)}$ in an asymptotically flat gauge at the “radiation zone”, far from the sources. This property ensures us direct comparison with ψ_4^{Num} by constructing $\psi_4^{(1)} + \psi_4^{(2)}$. In Sections IV.A-IV.C. we give an explicit and general prescription for the construction of second order gauge and tetrad invariant objects representing outgoing radiation. To do so we impose the waveform $\psi_I^{(2)}$ to be invariant under a “combined” transformation of both the coordinates and the tetrad frame to first and second order. The resulting second order invariant waveform can then be built up out of the original $\psi_4^{(2)}$ plus corrections (quadratic in the first order quantities) that cancel out the gauge and tetrad dependence of $\psi_4^{(2)}$. Finally, in Sec. V, along with a short summary, we discuss the astrophysical and numerical applications of our result. We end the paper with three appendices: Appendix A refers Sec. III.A and contains explicit formulas to compute the first order perturbative Newman-Penrose quantities (Weyl scalars, spin coefficients and perturbed tetrad) in terms of the first order metric perturbations needed to build up the source term in the wave equation for $\psi_I^{(2)}$. Appendix B refers to Sec. III.B and contains formulas to compute the second order spin coefficients in terms of the second order metric perturbations and product of first order perturbations needed, for instance, to build up $\psi_I^{(2)}$ in terms of initial data. Finally, in Appendix C we explicitly give the expressions to build up the gauge invariant waveform holding in the Schwarzschild limit case, i.e. for $a = 0$.

Notation: In this paper we use Refs. [30,13] conventions. Background quantities carry the (0) superindex if needed for clarity and are all explicitly given in the cited references, while superindices (1) and (2) mean pieces of *exclusively* first and second order respectively, for instance, we expand $\psi = \psi^{(0)} + \psi^{(1)} + \psi^{(2)} + \dots$

II. DECOUPLED EQUATIONS FOR HIGHER ORDER GRAVITATIONAL PERTURBATIONS

Let us consider the following two of the eight complex Bianchi identities written in the Newman-Penrose formalism (projected along a complex null tetrad) [31], Ch. 1.8 (see also the Appendix A)

$$\begin{aligned} & (D + 4\epsilon - \rho) \psi_4 - (\bar{\delta} + 4\pi + 2\alpha) \psi_3 + 3\lambda\psi_2 \\ & = 4\pi[(\bar{\delta} - 2\bar{\tau} + 2\alpha) T_{n\bar{m}} - (\Delta + 2\gamma - 2\bar{\gamma} + \bar{\mu}) T_{\bar{m}\bar{m}} - \lambda(T_{nl} + T_{m\bar{m}}) + \bar{\sigma}T_{nn} + \nu T_{l\bar{m}}], \end{aligned} \quad (2)$$

$$\begin{aligned} & (\delta + 4\beta - \tau) \psi_4 - (\Delta + 4\mu + 2\gamma) \psi_3 + 3\nu\psi_2 \\ & = 4\pi[(\bar{\delta} - \bar{\tau} + 2\bar{\beta} + 2\alpha) T_{nn} - (\Delta + 2\gamma + 2\bar{\mu}) T_{n\bar{m}} + \nu(T_{nl} + T_{m\bar{m}}) + \bar{\nu}T_{\bar{m}\bar{m}} - \lambda T_{nm}] \end{aligned} \quad (3)$$

and the following one out of the eighteen complex Ricci identities [31]

$$(\Delta + \mu + \bar{\mu} + 3\gamma - \bar{\gamma}) \lambda - (\bar{\delta} + 3\alpha + \bar{\beta} + \pi - \bar{\tau}) \nu + \psi_4 = 0. \quad (4)$$

Here $D = l^\mu \partial_\mu$, $\Delta = n^\mu \partial_\mu$, $\delta = m^\mu \partial_\mu$.

In what follows it is convenient to define the operators

$$\bar{d}_3 \doteq (\bar{\delta} + 3\alpha + \bar{\beta} + 4\pi - \bar{\tau}), \quad \bar{d}_4 \doteq (\Delta + 4\mu + \bar{\mu} + 3\gamma - \bar{\gamma}). \quad (5)$$

In order to find a decoupled equation for ψ_4 we operate with¹ $\bar{d}_4^{(0)}$ on Eq. (2), with $\bar{d}_3^{(0)}$ on Eq. (3), and then subtract to obtain

¹Here we use operators defined on the background instead of (5) for the sake of simplicity.

$$\begin{aligned}
& \left[\bar{d}_4^{(0)} (D + 4\epsilon - \rho) - \bar{d}_3^{(0)} (\delta + 4\beta - \tau) \right] \psi_4 \\
& + \left[\bar{d}_3^{(0)} (\Delta + 4\mu + 2\gamma) - \bar{d}_4^{(0)} (\bar{\delta} + 4\pi + 2\alpha) \right] \psi_3 \\
& - 3 \left[\bar{d}_3^{(0)} \nu - \bar{d}_4^{(0)} \lambda \right] \psi_2 \\
& = T[\text{matter}], \tag{6}
\end{aligned}$$

where $T[\text{matter}]$ is defined in Eq. (10) below.

In the above equation ψ_4, ψ_3, ν and λ vanish on the background, i.e. on the Kerr geometry, but so far this equation is exact, no perturbative expansion has been made yet. Let us now think how to use Eq. (6) in a perturbative scheme. In this context, the superindex (p) appearing in the formulae below stands for a sum over all perturbative orders from $p = 1$ up to $p = n - 1$ (i. e. $\sum_{p=1}^{n-1}$) where $n = 1, 2, \dots$ is an arbitrary order we want to study.

To fix ideas let us first discuss second order perturbations, $n = 2$. The procedure for higher order perturbations will be clearly analogous. We want to have an uncoupled equation for $\psi_4^{(2)}$. Since $\psi_4^{(0)} = 0$, the operator in the first bracket on the left hand side of Eq. (6) is needed to zeroth plus first order. The zeroth order acts on $\psi_4^{(2)}$ and generates the same wave operator as for the first order perturbations. The first order operator in the first bracket on the left hand side of Eq. (6) acts on $\psi_4^{(1)}$ and its result can be considered as generating an additional source term since it is supposed we have already solved for the first order perturbation problem previously. The second bracket on the left hand side of Eq. (6) can be considered as a pure source term as well since its zeroth order vanishes

$$\bar{d}_3^{(0)} (\Delta + 4\mu + 2\gamma)^{(0)} - \bar{d}_4^{(0)} (\bar{\delta} + 4\pi + 2\alpha)^{(0)} = 0,$$

(see Ref. [30] for an analogous proof) and then we have to consider $\psi_3^{(1)}$, i.e. only to first perturbative order (in general, to all lower perturbative orders than the one considered). The last bracket on the left hand side of Eq. (6) includes terms depending on $\nu^{(2)}$ and $\lambda^{(2)}$ since $\psi_2^{(0)} (= -M/(r - ia \cos \vartheta)^3)$, is non vanishing. To get rid of these second order spin coefficients we use Eq. (4) multiplied to the left by $\psi_2^{(0)}$

$$\left[\bar{d}_3^{(0)} \nu^{(n)} - \bar{d}_4^{(0)} \lambda^{(n)} \right] \psi_2^{(0)} = \psi_2^{(0)} \sum_{p=1}^{n-1} \left[(\bar{d}_3 - 3\pi)^{(n-p)} \nu^{(p)} - (\bar{d}_4 - 3\mu)^{(n-p)} \lambda^{(p)} \right] + \psi_2^{(0)} \psi_4^{(n)},$$

where we have made use of the pure zeroth order relations $\Delta^{(0)} \psi_2^{(0)} = -3\mu^{(0)} \psi_2^{(0)}$ and $\bar{\delta}^{(0)} \psi_2^{(0)} = -3\pi^{(0)} \psi_2^{(0)}$ coming from the Bianchi identities. The above result allow us again to write the terms depending on ψ_2 as source terms.

We finally obtain the equation that describes the n -th order perturbations

$$\left\{ \bar{d}_4^{(0)} (D + 4\epsilon - \rho)^{(0)} - \bar{d}_3^{(0)} (\delta + 4\beta - \tau)^{(0)} - 3\psi_2^{(0)} \right\} \psi_4^{(n)} = \mathcal{S}_4[\psi^{(n-p)}, \partial_t \psi^{(n-p)}] + T[\text{matter}], \tag{7}$$

where

$$\psi_4^{(n)} \doteq -(C_{\alpha\beta\gamma\delta} n^\alpha \bar{m}^\beta n^\gamma \bar{m}^\delta)^{(n)} \tag{8}$$

and the source terms are (where brackets represent operators)

$$\begin{aligned}
\mathcal{S}_4 = \sum_{p=1}^{n-1} \left\{ \right. & \left[\bar{d}_3^{(0)} (\delta + 4\beta - \tau)^{(n-p)} - \bar{d}_4^{(0)} (D + 4\epsilon - \rho)^{(n-p)} \right] \psi_4^{(p)} \\
& - \left[\bar{d}_3^{(0)} (\Delta + 4\mu + 2\gamma)^{(n-p)} - \bar{d}_4^{(0)} (\bar{\delta} + 4\pi + 2\alpha)^{(n-p)} \right] \psi_3^{(p)} \\
& + 3 \left[\bar{d}_3^{(0)} \nu^{(n-p)} - \bar{d}_4^{(0)} \lambda^{(n-p)} \right] \psi_2^{(p)} \\
& \left. - 3\psi_2^{(0)} \left[(\bar{d}_3 - 3\pi)^{(n-p)} \nu^{(p)} - (\bar{d}_4 - 3\mu)^{(n-p)} \lambda^{(p)} \right] \right\}, \tag{9}
\end{aligned}$$

and

$$T[\text{matter}] = \sum_{p=1}^{n-1} \left\{ \bar{a}_4^{(0)} \left[(\bar{\delta} - 2\bar{\tau} + 2\alpha)^{(n-p)} T_{n\bar{m}}^{(p)} - (\Delta + 2\gamma - 2\bar{\gamma} + \bar{\mu})^{(n-p)} T_{\bar{m}\bar{m}}^{(p)} \right] \right. \\ \left. + \bar{a}_3^{(0)} \left[(\Delta + 2\gamma + 2\bar{\mu})^{(n-p)} T_{n\bar{m}}^{(p)} - (\bar{\delta} - \bar{\tau} + 2\bar{\beta} + 2\alpha)^{(n-p)} T_{nn}^{(p)} \right] \right\}, \quad (10)$$

where $T_{n\bar{m}}^{(p)} = (T_{\mu\nu} n^\mu \bar{m}^\nu)^{(p)}$, $T_{\bar{m}\bar{m}}^{(p)} = (T_{\mu\nu} \bar{m}^\mu \bar{m}^\nu)^{(p)}$ and $T_{nn}^{(p)} = (T_{\mu\nu} n^\mu n^\nu)^{(p)}$. Note that in our formalism we have taken into account matter terms in order to be used in future computations including an orbiting particle or an accretion disk around a Kerr hole. By summing up over all n -orders in Eq. (7) one should be able to recover solutions to the full Einstein Equations.

Note also that if one wants to act on $\psi^{(n)} \doteq \rho^{-4} \psi_4^{(n)}$ rather than $\psi_4^{(n)}$ one should rescale all the terms (including the source) in Eq. (7) by a factor $2\rho^{-4}\Sigma$. After this rescaling, Eq. (7) takes the following familiar form

$$\widehat{T}\psi^{(n)} = 2\rho^{-4}\Sigma\{\mathcal{S}_4[\psi^{(n-p)}, \partial_t\psi^{(n-p)}] + T[\text{matter}]\}. \quad (11)$$

In Ref. [30] the wave operator was transformed to act on the field $\psi^{(1)} \doteq (\rho^{(0)})^{-4} \psi_4^{(1)}$ rather than $\psi_4^{(1)}$ (in order to achieve separability of the variables in the frequency domain) and takes the following form, in Boyer-Lindquist coordinates $(t, r, \vartheta, \varphi)$ and Kinnersley tetrad

$$\widehat{T} = \left[\frac{(r^2 + a^2)^2}{\Delta} - a^2 \sin^2 \vartheta \right] \partial_{tt} + \frac{4Mar}{\Delta} \partial_{t\varphi} - 4 \left[r + ia \cos \vartheta - \frac{M(r^2 - a^2)}{\Delta} \right] \partial_t \\ - \Delta^2 \partial_r (\Delta^{-1} \partial_r) - \frac{1}{\sin \vartheta} \partial_\vartheta (\sin \vartheta \partial_\vartheta) - \left[\frac{1}{\sin^2 \vartheta} - \frac{a^2}{\Delta} \right] \partial_{\varphi\varphi} \\ + 4 \left[\frac{a(r - M)}{\Delta} + \frac{i \cos \vartheta}{\sin^2 \vartheta} \right] \partial_\varphi + (4 \cot^2 \vartheta + 2), \quad (12)$$

where M is the mass of the black hole, a its angular momentum per unit mass, $\Sigma \equiv r^2 + a^2 \cos^2 \vartheta$, and $\Delta \equiv r^2 - 2Mr + a^2$. Note that if one wants to act on $\psi^{(2)} \doteq (\rho^{(0)})^{-4} \psi_4^{(2)}$ rather than $\psi_4^{(2)}$ in Eq. (6) then one should consistently rescale all the terms (including the source) by a factor $2(\rho^{(0)})^{-4}\Sigma$ (see Eq. (11)).

It is easy to show that a similar equation to (11) can be obtained for the Weyl scalar field ψ_0 , upon exchange of the tetrad vectors $l \leftrightarrow n$ and $\bar{m} \leftrightarrow m$. In this paper we will explicitly work with ψ_4 since it directly represents outgoing gravitational radiation. Since at every level of the hierarchy of perturbations we have the zeroth order wave operator acting on $\psi_4^{(n)}$ we could always use the method of full separations of variables. In this paper, however, we will not proceed so because we want our equations to be suitable for evolution in the time domain from given Cauchy data.

III. PRACTICAL ISSUES

A. Gauge choice and computation of the source

As we will show explicitly in the next Section, ψ_4 is neither invariant under first order coordinates transformations nor second order tetrad rotations. Thus, in order to integrate Eq. (11), one would have to evolve ψ in a fixed gauge (and tetrad) and then compute physical quantities, like radiated energy and waveform, in an asymptotically flat gauge. This sort of approach was followed in Ref. [8] to study second order perturbations of a Schwarzschild black hole in the Regge-Wheeler gauge which is a unique gauge that allows to invert expressions in terms of generic perturbations and thus recover the gauge invariance. There is not a generalization of the Regge-Wheeler gauge when studying perturbations of a Kerr hole, essentially because one cannot perform a simple multipole decomposition of the metric. Instead, Chrzanowski [32] found two convenient gauges that allowed him to invert the metric perturbations in terms of potentials Ψ_{IRG} or Ψ_{ORG} satisfying the same wave equations as the Weyl scalars $\rho^{-4}\psi_4$ or ψ_0 respectively.

In the *ingoing radiation* gauge (IRG)

$$h_{ll}^{(1)} = 0 = h_{ln}^{(1)} = 0 = h_{lm}^{(1)} = 0 = h_{\bar{m}\bar{m}}^{(1)}, \quad (13)$$

the homogeneous (for vacuum) metric components can be written, in the time domain, in terms of solutions to the wave equation for $\rho^{-4}\psi_4^{(1)}$ only, as follows

$$(h_{\mu\nu}^{(1)})_{IRG} = 2Re \left[\left\{ -l_\mu l_\nu (\delta + \bar{\alpha} + 3\beta - \tau)(\delta + 4\beta + 3\tau) - m_\mu m_\nu (D - \rho)(D + 3\rho) \right. \right. \\ \left. \left. + l_{(\mu} m_{\nu)} [(D + \bar{\rho} - \rho)(\delta + 4\beta + 3\tau) + (\delta - \bar{\alpha} + 3\beta - \bar{\pi} - \tau)(D + 3\rho)] \right\} (\Psi_{IRG}) \right] \quad (14)$$

where Re stands for the real part of the whole object to ensure that the metric be real [33,34] and we made the $\epsilon = 0$ choice. Note that in this gauge the metric potential has the property to be transverse ($h_{\mu\nu}^{(1)} l^\mu = 0$) and traceless ($h_{\mu}^{(1)\mu} = 0$) at the future horizon and past infinity. This is thus a suitable gauge to study gravitational radiation effects near the event horizon.

The complementary (adjoint) gauge to the ingoing radiation gauge is the *outgoing radiation gauge* (ORG),

$$h_{nn}^{(1)} = 0 = h_{ln}^{(1)} = 0 = h_{nm}^{(1)} = 0 = h_{n\bar{m}}^{(1)} = 0 = h_{m\bar{m}}^{(1)}. \quad (15)$$

where the metric potential has now the property to be transverse ($h_{\mu\nu}^{(1)} n^\mu = 0$) and traceless ($h_{\mu}^{(1)\mu} = 0$) at the past horizon and future infinity. It is then an example of a suitable asymptotically flat gauge to directly compute radiated energy and momenta at infinity (see Sec. III.C). In this gauge, the homogeneous metric components can be written in terms of solutions to the wave equation for $\psi_0^{(1)}$, as

$$(h_{\mu\nu}^{(1)})_{ORG} = 2Re \left[\rho^{-4} \left\{ -n_\mu n_\nu (\bar{\delta} - 3\alpha - \bar{\beta} + 5\pi)(\bar{\delta} - 4\alpha + \pi) - \bar{m}_\mu \bar{m}_\nu (\Delta + 5\mu - 3\gamma + \bar{\gamma})(\Delta + \mu - 4\gamma) \right. \right. \\ \left. \left. + n_{(\mu} \bar{m}_{\nu)} [(\bar{\delta} - 3\alpha + \bar{\beta} + 5\pi + \bar{\tau})(\Delta + \mu - 4\gamma) + (\Delta + 5\mu - \bar{\mu} - 3\gamma - \bar{\gamma})(\bar{\delta} - 4\alpha + \pi)] \right\} (\Psi_{ORG}) \right] \quad (16)$$

Note that Eqs. (13) (or (15)) are *four* conditions on the *real* part of the metric. Although (13) (or (16)) do not fix completely the gauge freedom, Chrzanowski metric choice given in Eq. (14) (or Eq. (16)), being a specific choice between all the possible solutions satisfying those conditions, *does uniquely fix* all of the extra freedom.

The potentials Ψ_{IRG} and Ψ_{ORG} fulfil the Teukolsky equation for $\rho^{-4}\psi_4$ and ψ_0 respectively. To determine them we can invert expressions Eqs. (13) or (15) and its time derivatives at the initial Cauchy surface to relate the potential to our first order initial data. Alternatively, one can use the relations of these potentials to gauge invariant objects like ψ_0 or $\rho^{-4}\psi_4$. For instance, in the IRG we can take the relation $\psi_0 = DDDD\Psi_{IRG}$ (See Eq. (5.28) of Ref. [34]) or in the ORG the adjoint relation $\psi_4 = \Delta\Delta\Delta\Psi_{ORG}$. Here we lower the order of the time derivatives of Ψ to first order ones by repeated use of the Teukolsky equation potentials fulfill (See, for instance, Eq. (5.20) of Ref. [34]). Since one can always make a mode decomposition of the φ dependence one ends up with a set of potential equations for $\Psi(r, \theta)$ and $\partial_t\Psi(r, \theta)$ at the initial time. Boundary conditions are chosen such that we obtain bounded solutions. The numerical integration of these equations is left for a forthcoming paper [42]. These solutions give us the initial data to integrate the wave equations and then build up metric perturbations from Eqs. (13) or (15). The imposition of initial data to ψ_4 and ψ_0 is discussed in the next subsection.

Finally, in order to integrate Eq. (11) we assumed the knowledge of the source term (9) since it depends only on first order perturbations. In practice, one solves the Teukolsky equation for $\psi_4^{(1)}$ (and / or $\psi_0^{(1)}$) and builds up metric perturbations. It then remains the task of writing all first order Newman-Penrose quantities in terms of $h_{\mu\nu}$. This is not a trivial task, so we give all the equations relating the Newman-Penrose fields to the metric perturbations in appendix A.

B. Imposition of initial data

To start the evolution one has to be able to impose initial data to the second order invariant waveform. We first note that, from its definition, we can write

$$\psi_4^{(2)} = -C_{n\bar{m}n\bar{m}}^{(2)} + \frac{1}{4}h_{nn}^{(1)}h_{m\bar{m}}^{(1)} (\psi_2^{(0)} + \bar{\psi}_2^{(0)}) - 2 \left(h_{ln}^{(1)} - \frac{1}{2}h_{m\bar{m}}^{(1)} \right) \psi_4^{(1)} - 2h_{n\bar{m}}^{(1)}\psi_3^{(1)}. \quad (17)$$

For the sake of definiteness we have used here Eq. (A1) choice of the first order tetrad, but it is clear that the above expression can be written in a generic tetrad. Besides, since we are going to build up the invariant $\psi_I^{(2)}$, any choice of the tetrad (and the gauge) leads to the same, correct, result.

In Ref. [26] we have completely expressed $\psi_4^{(1)}$ (and its time derivative) in terms of hypersurface data only. The expression²

$$C_{n\overline{m}n\overline{m}} = - \left[{}^{(3)}R_{ijkl} + 2K_{i[k}K_{l]j} \right] \hat{n}^i \hat{\overline{m}}^j \hat{n}^k \hat{\overline{m}}^l + 8N \left[K_{j[k,l]} + {}^{(3)}\Gamma_{j[k}^p K_{l]p} \right] \hat{n}^{[0\hat{\overline{m}}^j]} \hat{n}^{k\hat{\overline{m}}^l} - 4N^2 \left[{}^{(3)}R_{jl} - K_{jp}K_l^p + KK_{jl} - T_{jl} + \frac{1}{2}Tg_{jl} \right] \hat{n}^{[0\hat{\overline{m}}^j]} \hat{n}^{[0\hat{\overline{m}}^l]} \quad (18)$$

and its time derivative hold in general, to all order. Here $N = (-g^{tt})^{-1/2}$, $N^i = N^2 g^{ti}$, $\hat{n}^\mu = n^\mu + N^i n^t$ and $\hat{\overline{m}}^\mu = \overline{m}^\mu + N^i \overline{m}^t$. When we expand the above relation to a given perturbative order n , the proof given in Ref. [26] implies that ψ_4 and $\partial_t \psi_4$ will be independent on the lapse and shift of order n (but will depend, of course, on all lower perturbative orders of N and N^i).

To express our second order object $\psi_I^{(2)}$ in terms of the three-metric and the extrinsic curvature of the initial hypersurface we will proceed as in Ref. [26] taking now into account the additional terms, quadratic in the first order perturbations. We then find

$$C_{n\overline{m}n\overline{m}}^{(2)} = - \left[{}^{(3)}R_{ijkl} + 2K_{i[k}K_{l]j} \right]_{(2)} \hat{n}^i \hat{\overline{m}}^j \hat{n}^k \hat{\overline{m}}^l + 8N_{(0)} \left[K_{j[k,l]} + {}^{(3)}\Gamma_{j[k}^p K_{l]p} \right]_{(2)} \hat{n}^{[0\hat{\overline{m}}^j]} \hat{n}^{k\hat{\overline{m}}^l} - 4N_{(0)}^2 \left[{}^{(3)}R_{jl} - K_{jp}K_l^p + KK_{jl} - T_{jl} + \frac{1}{2}Tg_{jl} \right]_{(2)} \hat{n}^{[0\hat{\overline{m}}^j]} \hat{n}^{[0\hat{\overline{m}}^l]} + 8N_{(1)} \left[K_{j[k,l]} + {}^{(3)}\Gamma_{j[k}^p K_{l]p} \right]_{(1)} \hat{n}^{[0\hat{\overline{m}}^j]} \hat{n}^{k\hat{\overline{m}}^l} - 8N_{(0)}N_{(1)} \left[{}^{(3)}R_{jl} - K_{jp}K_l^p + KK_{jl} - T_{jl} + \frac{1}{2}Tg_{jl} \right]_{(1)} \hat{n}^{[0\hat{\overline{m}}^j]} \hat{n}^{[0\hat{\overline{m}}^l]} \quad (19)$$

Note that the first three terms have the same structure as in the first order case [for terms linear in $h_{ij}^{(2)}$ and $K_{ij}^{(2)}$.] There is not dependence on the second order lapse and shift, but $N_{(1)}$ and the perturbative shift now explicitly appear. To re-express them in terms of hypersurface data, we can make use of Eq. (14) and Appendix A expressions that relate all first order quantities to Ψ_{ORG} , directly expressible in terms of hypersurface data only as discussed before. And the same technique allow us to build up the additional quadratic terms occurring in $\psi_I^{(2)}$. Since the total $\psi_I^{(2)}$ was originally invariant, its final expression is not affected by the use of the a gauge choice (such as (14) or (16)) at an intermediate step.

For $\partial_t \psi_I^{(2)}$, the procedure is the same as before. We note that terms linear in $h_{ij}^{(2)}$ and $K_{ij}^{(2)}$ will have the same structure as in the first order case, so Eq. (3.2) of Ref. [26] applies upon change of the subindex (1) by (2). The additional terms, quadratic in the first order perturbations, can be directly written in terms of $\partial_t \Psi_{IRG}$ by taking the time derivative of Eq. (14) and Appendix A expressions.

In Appendix B we give an independent derivation relating $\psi_4^{(2)}$ to the four-geometry. We split

$$\psi_4^{(2)} \doteq \psi_{4L}^{(2)} + \psi_{4Q}^{(2)}, \quad (20)$$

where the first term on the right hand side is linear in the second order perturbations of the metric, i.e. $h_{\mu\nu}^{(2)}$ and is formally the same as $\psi_4^{(1)}$ replacing $h_{\mu\nu}^{(2)} \rightarrow h_{\mu\nu}^{(1)}$. The second term on the right hand side, i.e. $\psi_{4Q}^{(2)}$, accounts for the quadratic part in first order metric perturbations.

C. Radiated energy and momenta

The energy and momenta radiated at infinity to second perturbative order can be computed using the standard methods of linearized gravity (here $h_{\mu\nu}$ stands for $h_{\mu\nu}^{(1)} + h_{\mu\nu}^{(2)} + \dots$ defined in asymptotically flat coordinates at future null infinity). For outgoing waves [30]

²Note that the factor 8 appearing in front of the second bracket corrects an obvious misprint in Ref. [26]. This also applies to the Eq. (3.2) for $\partial_t \psi_4^{(1)}$.

$$\lim_{r \rightarrow \infty} \psi_4 = -\frac{1}{2}(\partial_t^2 h_{\hat{\vartheta}\hat{\vartheta}} - i\partial_t^2 h_{\hat{\vartheta}\hat{\varphi}}), \quad (21)$$

the total radiated energy per unit time ($u = t - r$) can thus be obtained from the Landau-Lifschitz pseudo tensor as

$$\frac{dE}{du} = \lim_{r \rightarrow \infty} \left\{ \frac{r^2}{4\pi} \int_{\Omega} d\Omega \left| \int_{-\infty}^u d\tilde{u} \psi_4(\tilde{u}, r, \vartheta, \varphi) \right|^2 \right\}, \quad d\Omega = \sin \vartheta \, d\vartheta \, d\varphi, \quad (22)$$

where we can consider $\psi_4 = \psi_4^{(1)} + \psi_4^{(2) AF} + \dots$

Note that Eq. (22) can be equivalently obtained by directly calculating the Bondi definition of the mass carried away by the gravitational radiation by imposing asymptotically flat conditions to the full Newman-Penrose quantities in a general vacuum spacetime. In this way, one can also compute the total linear momentum radiated at infinity per unit time along cartesian-like coordinates as [35]

$$\frac{dP_{\mu}}{du} = - \lim_{r \rightarrow \infty} \left\{ \frac{r^2}{4\pi} \int_{\Omega} d\Omega \tilde{l}_{\mu} \left| \int_{-\infty}^u d\tilde{u} \psi_4(\tilde{u}, r, \vartheta, \varphi) \right|^2 \right\}, \quad (23)$$

$$\tilde{l}_{\mu} = (1, -\sin \theta \cos \varphi, -\sin \theta \sin \varphi, -\cos \theta),$$

and the angular momentum carried away by the waves [36] can be obtained from

$$\frac{dJ_z}{du} = - \lim_{r \rightarrow \infty} \left\{ \frac{r^2}{4\pi} \operatorname{Re} \left[\int_{\Omega} d\Omega \left(\partial_{\varphi} \int_{-\infty}^u d\tilde{u} \psi_4(\tilde{u}, r, \vartheta, \varphi) \right) \left(\int_{-\infty}^u du' \int_{-\infty}^{u'} d\tilde{u} \bar{\psi}_4(\tilde{u}, r, \vartheta, \varphi) \right) \right] \right\}. \quad (24)$$

One can directly compute the second order correction to the energy and momentum radiated at \mathcal{J}^+ using $\psi_4^{(2)}$, provided one is working (to first order) in an asymptotically flat gauge (for instance, the outgoing radiation gauge). Eqs. (22)–(24), written in terms of the full, nonlinear ψ_4 , are covariant expressions, holding in any asymptotically flat spacetime. To first perturbative order, $\psi_4^{(1)}$ is directly gauge and tetrad invariant, so one can forget that the above equations had been obtained in an asymptotically flat gauge and think of them as gauge (and tetrad) invariant. We would like to have the same nice property to second perturbative order, but $\psi_4^{(2)}$ is not invariant. One should then build up a gauge (and tetrad) invariant waveform $\psi_I^{(2)}$ that, in an asymptotically flat gauge coincides with $\psi_4^{(2) AF}$. This will ensure us the direct use of Eqs. (22)–(24) in terms of our invariant object, i.e. $\psi_I^{(2)}$ given in Eq. (41).

IV. CONSTRUCTION OF THE SECOND ORDER COORDINATE AND TETRAD INVARIANT WAVEFORM

The general covariance (i.e. diffeomorphism invariance) of Einstein's theory of gravity guarantees the complete freedom in the choice of the spacetime coordinates (gauge) to describe physical phenomena. In the relativistic theory of perturbations one always introduces two spacetimes, the physical (perturbed) spacetime and an idealized (unperturbed) background. In this way the perturbations can be viewed as fields propagating on the background. Consequently, to compare any physical quantity in the perturbed spacetime with the same quantity in the unperturbed spacetime it is necessary to introduce a diffeomorphism about the pairwise identification points between the two manifolds. The arbitrariness in the choice of this point identification map introduces an additional freedom to the usual gauge freedom of general relativity and is at the origin of the *gauge problem* in perturbation theory [37]. A convenient way to deal with this gauge problem is to construct quantities which are invariant under a change of the identification map of the perturbed spacetime while the background coordinates are held fixed.

Invariance in the Newman-Penrose formalism has a more restrictive meaning than in the standard (metric) perturbation theory, since the introduction of a tetrad frame at every point of the spacetime now requires that any physical perturbation must be invariant not only under infinitesimal gauge transformations (GI), but also under infinitesimal rotations of the local tetrad frame (TI). In this Section we briefly review the basic concepts of (higher order) tetrad invariance and coordinate (gauge) invariance in the framework of the Newman-Penrose formalism. We start with our second order object $\psi_4^{(2)}$, which is neither invariant under first order changes of the coordinates nor under second order tetrad rotations. We then show how to build up a tetrad invariant object by adding to $\psi_4^{(2)}$ a conveniently chosen term, quadratic in the first order perturbations. In this way the new object will be invariant under the (6-parameter) tetrad rotations. The procedure for the construction of the totally invariant object, i.e. also under coordinate choices (4-parameters) is analogous, but algebraically more involved. The final result is a general prescription for constructing totally invariant (I) quantities directly related to the (outgoing) gravitational radiation.

A. Tetrad invariance

The 6-parameter group of homogeneous Lorentz transformations, which preserves the tetrad orthogonality relations $l_\mu n^\mu = -m_\mu \bar{m}^\mu = 1$ (and all other scalar products zero), can be decomposed into three Abelian subgroups:

- Null rotation of type (I) which leaves the l_μ unchanged:

$$\begin{aligned}\tilde{l}_\mu &\rightarrow l_\mu \\ \tilde{n}_\mu &\rightarrow n_\mu + a\bar{m}_\mu + \bar{a}m_\mu + a\bar{a}l_\mu, \\ \tilde{m}_\mu &\rightarrow m_\mu + al_\mu;\end{aligned}\tag{25}$$

- Null rotation of type (II), which leaves the n_μ unchanged:

$$\begin{aligned}\tilde{l}_\mu &\rightarrow l_\mu + b\bar{m}_\mu + \bar{b}m_\mu + b\bar{b}n_\mu, \\ \tilde{n}_\mu &\rightarrow n_\mu, \\ \tilde{m}_\mu &\rightarrow m_\mu + bn_\mu;\end{aligned}\tag{26}$$

- Boost and rotation of type (III):

$$\begin{aligned}\tilde{l}_\mu &\rightarrow Al_\mu, \\ \tilde{n}_\mu &\rightarrow A^{-1}n_\mu, \\ \tilde{m}_\mu &\rightarrow \exp(i\theta)m_\mu;\end{aligned}\tag{27}$$

where (a, b) are two complex functions and (A, θ) two real functions on the four dimensional manifold, hence the six arbitrary parameters. When these functions are taken to be infinitesimally small the above transformations can be expanded up to an arbitrary order and then applied to any Newman-Penrose quantity.

Under a combined tetrad rotation of classes I, II, and III

$$\widetilde{\psi}_4^{(2)} \rightarrow \psi_4^{(2)} + 2[(A - 1) - i\theta]\psi_4^{(1)} + 4\bar{a}\psi_3^{(1)} + 6\bar{a}^2\psi_2^{(0)}.\tag{28}$$

The idea here is to supplement $\psi_4^{(2)}$ with additional terms that make the whole object tetrad invariant. Since we have to add those ‘‘correcting’’ terms on both sides of the field equation (11), we will write them as powers of first order perturbations so they can be added to the source term (9). The first step towards constructing this quantity is to note that $(l^r)^2(m^\vartheta)^2\psi_4/[(l^r{}^{(0)})^2(m^\vartheta{}^{(0)})^2]$ is invariant under rotations of class III. The second order piece of this combination of fields is

$$\psi_4^{(2)} + 2\left(\frac{l^r{}^{(1)}}{l^r{}^{(0)}} + \frac{m^\vartheta{}^{(1)}}{m^\vartheta{}^{(0)}}\right)\psi_4^{(1)}.\tag{29}$$

Note that the second addend exactly compensates for the variation of class III of $\psi_4^{(2)}$ (proportional to the parameters $A - 1$ and θ in Eq. (28)). In addition one can easily check that the second term in (29) is also invariant under rotations of class I and II with the Kinnersley choice [30] of the zeroth order tetrad

$$\begin{aligned}(l^\mu)^{(0)} &= \left(\frac{r^2 + a^2}{\Delta}, 1, 0, \frac{a}{\Delta}\right), \\ (n^\mu)^{(0)} &= \frac{1}{2(r^2 + a^2 \cos^2 \vartheta)} (r^2 + a^2, -\Delta, 0, a), \\ (m^\mu)^{(0)} &= \frac{1}{\sqrt{2}(r + ia \cos \vartheta)} (ia \sin \vartheta, 0, 1, i/\sin \vartheta),\end{aligned}\tag{30}$$

since $l^r{}^{(1)}$, $m^\vartheta{}^{(1)}$ and $\psi_4^{(1)}$ are all invariant³ under rotations of class I and II. Still, the first term in (29) varies with respect to rotations of class I and II. To correct that we note that under combined rotations I, II, and III

³It is clear that we can write the tetrad invariant object in terms of a generic zeroth order tetrad by replacing in Eq. (32) $l^r{}^{(1)} \rightarrow l^r{}^{(1)} - m^r \bar{\psi}_1^{(1)}/(3\bar{\psi}_2^{(0)}) - \bar{m}^r \psi_1^{(1)}/(3\psi_2^{(0)})$ and $m^\vartheta{}^{(1)} \rightarrow m^\vartheta{}^{(1)} - l^\vartheta \psi_3^{(1)}/(3\psi_2^{(0)})$. We take the background tetrad (30) for the sake of simplicity.

$$\widetilde{\psi}_3^{(1)} \rightarrow \psi_3^{(1)} + 3\bar{\alpha}\psi_2^{(0)}. \quad (31)$$

This allows us to solve for $\bar{\alpha}$ and replace it into the new expression (its form suggested by the $\bar{\alpha}$ dependence in the transformation (28)) that supplement (29). [Note that this replacement is successful because ψ_3 vanishes to zeroth order.] Thus, the object,

$$\psi_4^{(2)} + 2\psi_4^{(1)} \left(\frac{l^r}{l^r} \frac{(1)}{(0)} + \frac{m^\vartheta}{m^\vartheta} \frac{(1)}{(0)} \right) - \frac{2}{3} \frac{\left(\psi_3^{(1)} \right)^2}{\psi_2^{(0)}}, \quad (32)$$

is second order tetrad invariant.

While the above combination is tetrad invariant, one can see from the general behavior of the Weyl scalars and spin coefficients in an asymptotically flat gauge (see, for instance Sec. VII of Ref. [13]), that the quadratic term we added does not vanish relative to $\psi_4^{(2)}$ for large r , i.e. goes like $\mathcal{O}(1/r)$ as well. In order to have the desired property that in the radiation zone the invariant object approaches $\psi_4^{(2) AF}$ (AF stands for an asymptotically flat gauge), we will subtract to (32) another quadratic part that both, cancels its added asymptotic behavior and is tetrad (and gauge) invariant in order to preserve the gained invariance of (32). Symbolically, if we call Q the quadratic part we added to ψ_4 in Eq. (32), we search for a

$$\psi_4^{(2)} \Big|_{TI} \doteq \psi_4^{(2)} + Q - Q_I^{AF} \quad (33)$$

A practical way to build up Q_I^{AF} is to use relations (16), i.e. the perturbed metric in the outgoing radiation gauge, which is an asymptotically flat gauge at infinity. In this gauge, we evaluate the quadratic part Q in (32) and once, re-expressed all in terms of Ψ_{ORG} via Eqs. (16), we can forget that we used the outgoing radiation gauge and see Q_I^{ORG} as a tetrad and gauge invariant object, since Ψ_{ORG} is totally invariant. In the outgoing radiation gauge $\psi_4^{(2)}$ (and $\psi_4^{(2)} \Big|_{TI}$) reduces to $\psi_4^{(2)} \Big|_L$ as can be directly deduced from the expressions given in Appendix B.

B. Gauge invariance

The meaning of gauge invariance under infinitesimal coordinate changes, to an arbitrary order in the perturbations, was explicitly elucidated in Ref. [38] following the approach of Ref. [39]. Locally, these gauge transformations are the 4-parameter group of the inhomogeneous Lorentz transformations. Up to second order in the perturbations an infinitesimal change of coordinates

$$\tilde{x}^\mu \rightarrow x^\mu + \varepsilon \xi_{(1)}^\mu + \frac{1}{2} \varepsilon^2 (\xi_{(1); \nu}^\mu \xi_{(1)}^\nu + \xi_{(2)}^\mu), \quad (34)$$

where $\xi_{(1)}^\mu$ and $\xi_{(2)}^\mu$ are two independent arbitrary vector fields and ε a small (perturbative) parameter, produces the following effect on the first and second order perturbations of any quantity Φ (scalar, vector or tensor field) that we assume can be expanded as $\Phi^{(0)} + \Phi^{(1)} + \Phi^{(2)} + \dots$

$$\tilde{\Phi}^{(1)} \rightarrow \Phi^{(1)} + \mathcal{L}_{\xi_{(1)}} \Phi^{(0)}, \quad (35)$$

$$\tilde{\Phi}^{(2)} \rightarrow \Phi^{(2)} + \mathcal{L}_{\xi_{(1)}} \Phi^{(1)} + \frac{1}{2} (\mathcal{L}_{\xi_{(1)}}^2 + \mathcal{L}_{\xi_{(2)}}) \Phi^{(0)} \quad (36)$$

where, for the sake of completeness we recall here explicitly the basic coordinate expressions of the Lie derivative along a vector field ξ^μ ,

$$\begin{aligned} \mathcal{L}_\xi \Phi &= \Phi_{, \mu} \xi^\mu, \text{ if } \Phi \text{ is a scalar;} \\ \mathcal{L}_\xi \Phi^\nu &= \Phi^\nu_{, \mu} \xi^\mu - \xi^\nu_{, \mu} \Phi^\mu, \text{ if } \Phi^\nu \text{ is a vector;} \\ \mathcal{L}_\xi \Phi_{\alpha\beta} &= \Phi_{\alpha\beta, \mu} \xi^\mu + \xi^\mu_{, \alpha} \Phi_{\mu\beta} + \xi^\mu_{, \beta} \Phi_{\alpha\mu}, \text{ if } \Phi_{\alpha\beta} \text{ is a tensor.} \end{aligned} \quad (37)$$

Note that from transformation (35) it follows that all Newman-Penrose quantities that vanishes on the background (or more precisely satisfy $\mathcal{L}_{\xi_{(1)}} \Phi^{(0)} = 0$), like $\psi_0^{(1)}$, $\psi_4^{(1)}$, $\psi_3^{(1)}$, $k^{(1)}$, $\sigma^{(1)}$, $\lambda^{(1)}$, $\nu^{(1)}$, are first order gauge invariant (GI). Transformation (36), however, states that none of these Newman-Penrose quantities, to the second order in the perturbations, are gauge invariant, since $\mathcal{L}_{\xi_{(1)}} \Phi^{(1)} \neq 0$. Thus, none of the interesting Newman-Penrose quantities

that are tetrad invariant (TI) and gauge invariant to the first order are also invariant to the second order in the perturbations. In particular, second order gauge invariance requires that the quantity vanishes to zeroth and to first perturbative order.

Explicitly, for the scalar field ψ_4 we have

$$\widetilde{\psi_4^{(2)}} \rightarrow \psi_4^{(2)} + \frac{\partial \psi_4^{(1)}}{\partial x^\mu} \xi_{(1)}^\mu. \quad (38)$$

Hence we see that the vanishing of $\psi_4^{(0)}$ ensures that $\psi_4^{(2)}$ will be gauge invariant under “pure” second order changes of coordinates, but since $\psi_4^{(1)}$ will in general depend on all four coordinates, $\psi_4^{(2)}$ will *not* be gauge invariant under *first* order changes of the coordinates.

In order to apply similar techniques to those we used to construct a tetrad invariant object now in the coordinates context, i. e. by “correcting” $\psi_4^{(2)}$ with products of first order quantities, we will make use of the following Lemma

Lemma: *The product of the first order pieces $T^{(1)}P^{(1)}$ of two tensors (that can be expanded into perturbations) transforms under a first plus second order gauge change, given by Eq. (34), as the product of the first order transformed quantities individually.*

$$(T^{(1)}\widetilde{P}^{(1)}) \rightarrow (T^{(1)} + \mathcal{L}_{\xi_{(1)}}T^{(0)}) (P^{(1)} + \mathcal{L}_{\xi_{(1)}}P^{(0)})$$

Proof: Let T and P be two general tensor fields. Apply the first plus second order transformation (36) to the product and consider second order pieces, then

$$(\widetilde{TP})^{(2)} \rightarrow (TP)^{(2)} + \mathcal{L}_{\xi_{(1)}}(TP)^{(1)} + \frac{1}{2}(\mathcal{L}_{\xi_{(1)}}^2 + \mathcal{L}_{\xi_{(2)}})(TP)^{(0)},$$

or more explicitly

$$\begin{aligned} (T^{(2)}P^{(0)} + T^{(1)}\widetilde{P}^{(1)} + T^{(0)}P^{(2)}) &\rightarrow (T^{(2)}P^{(0)} + T^{(1)}P^{(1)} + T^{(0)}P^{(2)}) + \mathcal{L}_{\xi_{(1)}}(T^{(1)}P^{(0)} + T^{(0)}P^{(1)}) \\ &\quad + \frac{1}{2}(\mathcal{L}_{\xi_{(1)}}^2 + \mathcal{L}_{\xi_{(2)}})(T^{(0)}P^{(0)}). \end{aligned}$$

We now apply the same transformation (36) to the products $P^{(0)}T$ and $T^{(0)}P$ to obtain

$$P^{(0)}\widetilde{T}^{(2)} \rightarrow P^{(0)}T^{(2)} + P^{(0)}\mathcal{L}_{\xi_{(1)}}(T^{(1)}) + \frac{1}{2}P^{(0)}(\mathcal{L}_{\xi_{(1)}}^2 + \mathcal{L}_{\xi_{(2)}})(T)^{(0)}$$

similarly

$$T^{(0)}\widetilde{P}^{(2)} \rightarrow T^{(0)}P^{(2)} + T^{(0)}\mathcal{L}_{\xi_{(1)}}(P^{(1)}) + \frac{1}{2}T^{(0)}(\mathcal{L}_{\xi_{(1)}}^2 + \mathcal{L}_{\xi_{(2)}})(P)^{(0)}.$$

Upon subtraction of the last two expressions from the first one, we obtain

$$T^{(1)}\widetilde{P}^{(1)} \rightarrow T^{(1)}P^{(1)} + T^{(1)}\mathcal{L}_{\xi_{(1)}}(P^{(0)}) + P^{(1)}\mathcal{L}_{\xi_{(1)}}(T^{(0)}) + \mathcal{L}_{\xi_{(1)}}(T^{(0)})\mathcal{L}_{\xi_{(1)}}(P^{(0)}). \quad (39)$$

This proves our Lemma. An obvious corollary is the case when both fields are gauge invariant, i.e. $\mathcal{L}_{\xi_{(1)}}(T^{(0)}) = 0$ and $\mathcal{L}_{\xi_{(1)}}(P^{(0)}) = 0$ this generates a second order quantity that is first and second order gauge (coordinate) invariant.

To construct a second order gauge invariant waveform $\psi_{4\,GI}^{(2)}$ we can then use the same techniques as in the previous subsection. It is convenient now to start from our tetrad invariant object, as defined in Eq. (33). Under a first order coordinates change $\psi_{4\,TI}^{(2)}$ transform as

$$\widetilde{\psi_{4\,TI}^{(2)}} \rightarrow \psi_{4\,TI}^{(2)} + \psi_{4,\mu}^{(1)}\xi_{(1)}^\mu + 2\psi_4^{(1)} \left(\frac{l_{,\mu}^r{}^{(0)}\xi_{(1)}^\mu - \xi_{(1),\mu}^r l^{\mu(0)}}{l^r{}^{(0)}} + \frac{m_{,\mu}^\vartheta{}^{(0)}\xi_{(1)}^\mu - \xi_{(1),\mu}^\vartheta m^{\mu(0)}}{m^\vartheta{}^{(0)}} \right) \quad (40)$$

where we made use of the properties expressed in Eqs (38) and (39).

As in Section III.A, the idea here is to add to $\psi_4^{(2)}$ terms quadratic in the first order perturbations in order to make the whole object coordinate invariant⁴ while preserving its tetrad invariance. The procedure can be summarized as follows,

Prescription: The first step is to invert the coordinate transformations of first order quantities for the gauge vectors $\xi_{(1)}^\mu$. We shall denote this first order combination by the *boldface* vector: $\boldsymbol{\xi}_{(1)}^\mu$, i.e. $\xi_{(1)}^\mu = \widetilde{\xi}_{(1)}^\mu - \xi_{(1)}^\mu$. Making the replacement $\xi_{(1)}^\mu \rightarrow -\boldsymbol{\xi}_{(1)}^\mu$ into Eq. (40) above generates a totally invariant object. Still from all the possible invariant objects we want those whose quadratic term do not contribute to the radiation in an asymptotically flat gauge (AF). As we discussed at the end of Sec. IV.A, this ensures us a simple interpretation of the invariant ψ_I regarding radiated energy and waveforms. Since Eq. (40) is linear in $\xi_{(1)}^\mu$, subtracting the quadratic term in an asymptotically flat gauge will be equivalent to make the following replacement $\xi_{(1)}^\mu \rightarrow \boldsymbol{\xi}_{(1)}^{AF} - \xi_{(1)}^\mu$. As we discussed before, a practical way to evaluate $\boldsymbol{\xi}_{(1)}^{AF\mu}$ and keep the tetrad and coordinate invariance is to use the outgoing radiation gauge (Eq. (16)) and consider the final expression in terms of Ψ_{ORG} as a totally invariant expression regardless its derivation with a choice of the first order gauge and tetrad.

We recall here that $\psi_4^{(2)}$ and of course also terms quadratic in the first order perturbations are already invariant under pure second order coordinate transformations, labeled by $\xi_{(2)}^\mu$. Finally, our invariant waveform can then be symbolically expressed as

$$\begin{aligned} \psi_{4I}^{(2)} \doteq \psi_{4TI}^{(2)} + \psi_{4,\mu}^{(1)} \left(\boldsymbol{\xi}_{(1)}^{\mu ORG} - \boldsymbol{\xi}_{(1)}^\mu \right) + 2\psi_4^{(1)} \left[\frac{l_{,\mu}^{r(0)} \left(\boldsymbol{\xi}_{(1)}^{\mu ORG} - \boldsymbol{\xi}_{(1)}^\mu \right) - l^{\mu(0)} \left(\boldsymbol{\xi}_{(1),\mu}^{r ORG} - \boldsymbol{\xi}_{(1),\mu}^r \right)}{l^{r(0)}} \right. \\ \left. + \frac{m_{,\mu}^{\vartheta(0)} \left(\boldsymbol{\xi}_{(1)}^{\mu ORG} - \boldsymbol{\xi}_{(1)}^\mu \right) - m^{\mu(0)} \left(\boldsymbol{\xi}_{(1),\mu}^{\vartheta ORG} - \boldsymbol{\xi}_{(1),\mu}^{\vartheta} \right)}{m^{\vartheta(0)}} \right]. \end{aligned} \quad (41)$$

C. Construction of the second order invariant waveform

The above prescription is conceptually very simple. However, in practice, to find $\boldsymbol{\xi}_{(1)}^t$ and $\boldsymbol{\xi}_{(1)}^\varphi$ brings some technical complications. The first remark is that the procedure is not unique. We have a big choice of first order objects (all Newman-Penrose quantities, metric, extrinsic curvature, etc) to build up $\boldsymbol{\xi}_{(1)}^\mu$. In fact, one can easily see that the ambiguity to generate an invariant waveform has to be present since one can always add products of first order invariant objects to generate a new second order invariant object. The requirement that the quadratic correction must not influence the asymptotic behavior greatly reduces this ambiguity. In fact, physical quantities such as the radiated energy and observed waveform, defined in an asymptotically flat region, are uniquely defined by this method, since the differences introduced by different asymptotically flat coordinates vanish with a higher power of r . We thus, give an explicit object in order to be able to make comparisons with, for instance, full numerical results that directly compute the covariant object ψ_4 . Below we give a simple choice of $\boldsymbol{\xi}_{(1)}^\mu$, in order to construct $\psi_{4I}^{(2)}$ that is valid for perturbations of Kerr black holes, i.e. $a \neq 0$. In Appendix C we give another choice for the case of a Schwarzschild background.

In the rest of this subsection, to simplify the notation, we drop the subscript (1) from the first order gauge vectors $\boldsymbol{\xi}^\mu$ since we will never refer to the second order gauge vectors. The $\boldsymbol{\xi}^r$ and $\boldsymbol{\xi}^\vartheta$ components can be easily found from the variations of the tetrad invariant Weyl scalar $\psi_2^{(1)}$,

$$\widetilde{\psi_2^{(1)}} \rightarrow \psi_2^{(1)} + \boldsymbol{\xi}^r \partial_r \psi_2^{(0)} + \boldsymbol{\xi}^\vartheta \partial_\vartheta \psi_2^{(0)}, \quad (42)$$

and of its complex conjugate $\overline{\psi_2^{(1)}}$,

$$\boldsymbol{\xi}^r = -\frac{1}{6M} \left[\frac{\overline{\psi_2^{(1)}}}{\overline{\rho^4}} + \frac{\psi_2^{(1)}}{\rho^4} \right], \quad (43)$$

⁴A similar procedure was adopted to generate second order gauge invariants in the Moncrief's formulation of Schwarzschild black hole perturbations [40].

$$\xi^\vartheta = -\frac{1}{6M(ia \sin \vartheta)} \left[\frac{\bar{\psi}_2^{(1)}}{\bar{\rho}^4} - \frac{\psi_2^{(1)}}{\rho^4} \right]. \quad (44)$$

The same techniques cannot be straightforwardly applied to find the other two components ξ^t and ξ^φ . The origin of the problem can be traced back to the fact that the Kerr metric has two two killing vectors along ∂_t and ∂_φ , and thus one can never find local, first order quantities that vary with ξ^t or ξ^φ , but only with the derivatives of them. Explicitly, using the variations of the metric and extrinsic curvature components (which are tetrad invariant quantities), we find (here background fields are unlabeled)

$$\begin{aligned} \xi_{,t}^t &= \frac{g_{\varphi\varphi}(h_{tt}^{(1)} + g_{tt,r}\xi^r + g_{tt,\vartheta}\xi^\vartheta) - 2g_{t\varphi}(h_{t\varphi}^{(1)} + g_{t\varphi,r}\xi^r + g_{t\varphi,\vartheta}\xi^\vartheta + g_{t\varphi}\xi_{,\varphi}^\varphi + g_{tt}\xi_{,\varphi}^t)}{2(g_{t\varphi}^2 - g_{tt}g_{\varphi\varphi})}, \\ \xi_{,r}^t &= \frac{g_{\varphi\varphi}(h_{tr}^{(1)} + g_{rr}\xi_{,t}^r) - g_{t\varphi}(h_{r\varphi}^{(1)} + g_{rr}\xi_{,\varphi}^r)}{g_{t\varphi}^2 - g_{tt}g_{\varphi\varphi}}, \\ \xi_{,\vartheta}^t &= -\frac{(h_{t\vartheta}^{(1)} + g_{\vartheta\vartheta}\xi_{,t}^\vartheta + g_{t\varphi}\xi_{,\vartheta}^\varphi)}{g_{tt}}, \\ \xi_{,\varphi}^t &= -\frac{(h_{\varphi\varphi}^{(1)} + g_{\varphi\varphi,r}\xi^r + g_{\varphi\varphi,\vartheta}\xi^\vartheta + 2g_{\varphi\varphi}\xi_{,\varphi}^\varphi)}{2g_{t\varphi}}, \end{aligned} \quad (45)$$

and

$$\begin{aligned} \xi_{,t}^\varphi &= \frac{2g_{tt}(h_{t\varphi}^{(1)} + g_{t\varphi,r}\xi^r + g_{t\varphi,\vartheta}\xi^\vartheta + g_{t\varphi}\xi_{,\varphi}^\varphi + g_{tt}\xi_{,\varphi}^t) - g_{t\varphi}(h_{tt}^{(1)} + g_{tt,r}\xi^r + g_{tt,\vartheta}\xi^\vartheta)}{2(g_{t\varphi}^2 - g_{tt}g_{\varphi\varphi})}, \\ \xi_{,r}^\varphi &= \frac{g_{tt}(h_{r\varphi}^{(1)} + g_{rr}\xi_{,\varphi}^r) - g_{t\varphi}(h_{tr}^{(1)} + g_{rr}\xi_{,t}^r)}{g_{t\varphi}^2 - g_{tt}g_{\varphi\varphi}}, \\ \xi_{,\vartheta}^\varphi &= -\frac{K_{\vartheta\vartheta}^{(1)}}{2K_{\varphi\vartheta}}, \\ \xi_{,\varphi}^\varphi &= -\frac{(K_{r\varphi}^{(1)} + K_{\varphi r,r}\xi^r + K_{\varphi r,\vartheta}\xi^\vartheta + K_{\varphi r}\xi_{,r}^r)}{K_{\varphi r}}. \end{aligned} \quad (46)$$

Thus, to find ξ^t and ξ^φ one has to integrate their four derivatives over the spacetime. This can be performed like the integration of a potential in four dimensions. For that one has to verify the integrability conditions. In practice, since we are going to compute differences of these vectors, with respect to the asymptotically flat ones, the existence of the ξ^t and ξ^φ components are assumed a priori and they are related to the existence of the outgoing radiation gauge proved in Ref. [32]. As a consequence of these integrals on first order fields, the resulting waveform will be nonlocal, but this carries no further consequences since in solving the second order perturbations we assumed first order ones to be completely known. Notably, the evolution equation for the second order perturbations is *local*. In fact, only derivatives of ξ^t and ξ^φ enter in building up the source

$$\widehat{\mathcal{T}}[\psi_I^{(2)}] = S_I, \quad \psi_I^{(2)} \doteq (\rho^{(0)})^{-4} \psi_4^{(2)} I, \quad (47)$$

where the source term (as can be derived from Eq. (7)) is now

$$\begin{aligned} S_I &= 2(\rho^{(0)})^{-4} \Sigma \left\{ \mathcal{S}_4[\psi_4^{(1)}] + T[\text{matter}] \right\} \\ &+ \widehat{\mathcal{T}} \left[2\psi^{(1)} \left(\frac{l^r{}^{(1)} - l_{ORG}^r{}^{(1)}}{l^r{}^{(0)}} + \frac{m^\vartheta{}^{(1)} - m_{ORG}^\vartheta{}^{(1)}}{m^\vartheta{}^{(0)}} \right) - \frac{2 \left(\psi_3^{(1)} - \psi_3^{(1) ORG} \right)^2}{(\rho^{(0)})^4 \psi_2^{(0)}} \right] \\ &+ \widehat{\mathcal{T}} \left[\psi_{,\mu}^{(1)} \xi^\mu{}_{(1)} + 2\psi^{(1)} \left(\frac{l^r{}_{,\mu}{}^{(0)} \xi^\mu{}_{(1)} - \xi_{,\mu}^r{}_{(1)} l^{\mu}{}^{(0)}}{l^r{}^{(0)}} + \frac{m^\vartheta{}_{,\mu}{}^{(0)} \xi^\mu{}_{(1)} - \xi_{,\mu}^\vartheta{}_{(1)} m^{\mu}{}^{(0)}}{m^\vartheta{}^{(0)}} \right) \right], \end{aligned} \quad (48)$$

here $\xi^\mu \doteq \xi_{(1)}^{\mu ORG} - \xi_{(1)}^\mu$.

While the evolution is local, we need to compute the waveform at least on the initial hypersurface and then at the observer location (to compute, for instance, the radiated energy). At $t = 0$, after mode decomposition in the φ coordinate, we have

$$\xi^i = \sum_{m \neq 0} \frac{(\xi_{,\varphi}^i - \xi_{,\varphi}^{i \text{ ORG}})_m e^{im\varphi}}{im} + \int dr (\xi_{,r}^i - \xi_{,r}^{i \text{ ORG}}) + \int d\vartheta (\xi_{,\vartheta}^i - \xi_{,\vartheta}^{i \text{ ORG}}) - \int dr d\vartheta (\xi_{,r\vartheta}^i - \xi_{,r\vartheta}^{i \text{ ORG}}) + c^i, \quad (50)$$

where $i = (t, \varphi)$ and the same equation holds for the observer at a fixed r_{obs} , exchanging the roles of r and t .

Note the presence of the integration constants c^t and c^φ . They represent first order changes in the origin of time and azimuthal angle. This problem was already found in Ref. [8] and there it was given a method to fix ‘‘a posteriori’’ the value of the constants. In Section IV.B we generalize the procedure given in Ref. [8] and explicitly write the integrals that are necessary to fix the constants c^t and c^φ .

In order to compute the totally invariant second order waveform $\psi_{4 \text{ Ic}}^{(2)}$ we must fix the constants c_t and c_φ . We can generalize the gauge fixing prescription given in Ref. [7] and define ‘‘a posteriori’’ the value of the constants

$$c^t = \frac{\int_{-\infty}^{\infty} dt \dot{\psi}_4^{(1)} \psi_{4 \text{ I}}^{(2)} \int_{-\infty}^{\infty} dt (\partial_\varphi \psi_4^{(1)})^2 - \int_{-\infty}^{\infty} dt \partial_\varphi \psi_4^{(1)} \psi_{4 \text{ I}}^{(2)} \int_{-\infty}^{\infty} dt \dot{\psi}_4^{(1)} \partial_\varphi \psi_4^{(1)}}{\int_{-\infty}^{\infty} dt (\dot{\psi}_4^{(1)})^2 \int_{-\infty}^{\infty} dt (\partial_\varphi \psi_4^{(1)})^2 - \int_{-\infty}^{\infty} dt \dot{\psi}_4^{(1)} \partial_\varphi \psi_4^{(1)} \int_{-\infty}^{\infty} dt \dot{\psi}_4^{(1)} \partial_\varphi \psi_4^{(1)}}, \quad (51)$$

$$c^\varphi = \frac{\int_{-\infty}^{\infty} dt \dot{\psi}_4^{(1)} \partial_\varphi \psi_4^{(1)} \int_{-\infty}^{\infty} dt \dot{\psi}_4^{(1)} \psi_{4 \text{ I}}^{(2)} - \int_{-\infty}^{\infty} dt \partial_\varphi \psi_4^{(1)} \psi_{4 \text{ I}}^{(2)} \int_{-\infty}^{\infty} dt (\dot{\psi}_4^{(1)})^2}{\int_{-\infty}^{\infty} dt (\dot{\psi}_4^{(1)})^2 \int_{-\infty}^{\infty} dt (\partial_\varphi \psi_4^{(1)})^2 - \int_{-\infty}^{\infty} dt \dot{\psi}_4^{(1)} \partial_\varphi \psi_4^{(1)} \int_{-\infty}^{\infty} dt \dot{\psi}_4^{(1)} \partial_\varphi \psi_4^{(1)}}, \quad (52)$$

We can then construct the ‘‘c-invariant’’ waveform

$$\psi_{4 \text{ Ic}}^{(2)} = \psi_{4 \text{ I}}^{(2)} - (c^t \partial_t + c^\varphi \partial_\varphi) \psi_{4 \text{ I}}^{(1)}, \quad (53)$$

This procedure amounts to gauge fixing the zero of time and of the azimuthal angle in such a way that the integrals in the numerators of Eqs. (51) and (52) vanish. In order to be able to compare the perturbative results with the full numerical ones it is crucial that one is able to perform the same origin of coordinates fixing. Note that we can also fix these constants at the initial hypersurface $t = 0$. The same expressions (51)-(52) apply changing the integrations in time by integrations in r .

V. SUMMARY AND DISCUSSION

In this paper we presented a gauge and tetrad invariant framework for studying the evolution of general second order perturbations about a rotating black hole. To do so, we first uncoupled second (and higher) order perturbations of Kerr black holes for the Weyl scalar ψ_4 , that directly represents the outgoing gravitational radiation, and found that the perturbed outgoing radiation field $\psi_4^{(n)}$ fulfils a single Teukolsky-like equation (see Eq. (11)) with the same wave operator as for the first order perturbations [30], acting on the left hand side and an additional source term written as products of lower order perturbations on the right hand side of the equation. We note, however, that $\psi_4^{(2)}$ is neither tetrad nor *first order* coordinate (gauge) invariant. It is only invariant under purely *second* order changes of coordinates, simply because ψ_4 vanishes on the background (Kerr metric). Invariant objects to describe second perturbations lead us to reliable physical answers without having to face gauge difficulties. Hence, we explicitly show that it is always possible to correct $\psi_4^{(2)}$ in order to build up a complete second order invariant waveform $\psi_{4 \text{ I}}^{(2)}$ (i. e. invariant under both tetrad rotations and infinitesimal coordinates transformations) that gives a measure of the outgoing gravitational radiation. This is done in Sec. IV where we give a general *prescription* to produce the result expressed in Eq. (41). We also show that the same equation as (11), with a ‘‘corrected’’ source term, is now satisfied by $\psi_{4 \text{ I}}^{(2)}$ (see Eq. (47)). A number of interesting conceptual and technical issues raised from this computation, like the appearance of nonlocalities in the definition of the gauge invariant waveform when we want to relate it to known first order objects and its non uniqueness. Seen in retrospective, our method of generating a gauge invariant object is like a machine that transforms any (first order) gauge into an asymptotically flat one, in particular, into the outgoing radiation gauge. In fact, in this gauge we have $(\psi_4^{(2)})^{\text{ORG}} = (\psi_{4 \text{ L}}^{(2)})^{\text{ORG}} = (\psi_{4 \text{ I}}^{(2)})^{\text{ORG}} = \psi_{4 \text{ I}}^{(2)}$. This fits into Bardeen’s [41] interpretation of a gauge independent quantity and suggest to work in the outgoing radiation gauge as a particularly simple way of dealing with the numerical integration of the second order equations [42]. In

the language of Eq. (36) we see that the process of building up ψ_I is like subtracting the first order piece to ψ_4 . Our gauge invariant object, ψ_I , is not the second order term of a series expansion of ψ_4 , but it can be related to $psi_4^{(2)}$ in an asymptotically flat gauge.

The spirit of this work has been to show that there exists a gauge invariant way to deal with second order perturbations in the more general case of a rotating black hole and to provide theoretical support to the numerical integration of the second order perturbation problem. In order to implement such integration of Eq. (47) we proceed as follows: We assume that on an initial hypersurface we know the first and second order perturbed metric and extrinsic curvature. We then solve the first order problem, i.e. solve the standard Teukolsky equation for $\psi_4^{(1)}$ (and for $\psi_0^{(1)}$). Next we build up the perturbed metric coefficients in, for instance, the outgoing radiation gauge (15). The perturbed spin coefficients are now given by expression (A4) and the perturbed covariant basis by (A2). Those are all the necessary elements to build up the effective source term appearing on the right hand side of our evolution equation, as explained in Section III.A. It is worth to note here that from the analysis of the asymptotic behavior of the different Newman-Penrose quantities [13] involved in the source, one can see that at infinity the envelope of (the oscillating) S_4 is at least of $\mathcal{O}(r^{-2})$, which guarantees the convergence of the integration of Eq. (47).

The other piece of information that we need in order to integrate Eq. (47) is $\psi_I^{(2)}$ on the initial hypersurface. This is explained in Section III.B. We also need to use in this case Eq. (20) and the expressions given in Appendix B. For the computation of the radiated energy and momentum one uses Eqs. (22) and (23). The advantage of this procedure is that we can now use the same (2+1)-dimensional code for evolving the first order perturbations [19] by adding a source term. In fact, the background (Kerr) metric allows a decomposition into axial modes, i.e. the variable φ . A mode decomposition of all quantities involved in the second order evolution equation can be trivially performed (note that in the source, involving quadratic terms in the first order perturbations one has to include a double sum over modes, let us say, m and m'). In the time domain no further mode decomposition (i.e. in ℓ -multipole) of the source term is practical.

An important application of the formalism presented in this paper [42] is to reproduce the results obtained in Refs. [6] (for the nonrotating case and the multipole $\ell = 2$). The complexity of the calculations in the standard Zerilli formalism that would follow from considering the sum over all multipoles can be notably simplified in the Newman-Penrose formalism. We can thus also study the $\ell = 4$ multipole of the radiation and not only test the efficiency of our formalism, but also make a more detailed comparison with full numerical results. The next step is to extend the numerical computation to the more interesting case of rotating black holes. The numerical integration of Eq. (47) will be relevant not only for establishing the range of validity of the collision parameters in the close limit approximation, but (hopefully) to produce a more precise computation of the gravitational radiation. Direct comparison with the existing codes for numerical integration of the full nonlinear Einstein equations is possible [43].

Following the steps described in this paper, upon exchange of the null directions $l \leftrightarrow n$ and $\bar{m} \leftrightarrow m$, it is straightforward to write the corresponding equations for ψ_0 in case one wants to have a description in terms of ingoing waves. This would allow to study the influence of gravitational radiation on the horizon of a rotating black hole, critical collapse and also phenomena in their interior, like the mass-inflation. We studied in detail only gravitational perturbations, but it seems straightforward to generalize our method to scalar and vector perturbations. We also note that, although we have focused our attention on the problem of colliding black holes, the second order perturbative formalism developed in this paper can be easily generalized to any Petrov type D (or even type II) background metric and thus can be applied to study other interesting astrophysical scenarios as nonrotating neutron stars and cosmology.

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APPENDIX A: FIRST ORDER NEWMAN-PENROSE QUANTITIES

Throughout this Appendix, to simplify the notation, we omit the superscript (0) on the background quantities, while all first order quantities are denoted with the superscript (1) with the exception of the first order metric perturbation that we simply denote as $h_{\mu\nu}$.

Let us first note that the perturbed null tetrad can be represented by [44]

$$\begin{aligned}
l^{\mu(1)} &= -\frac{1}{2}h_{ll}n^\mu, \\
n^{\mu(1)} &= -\frac{1}{2}h_{nn}l^\mu - h_{nl}n^\mu, \\
m^{\mu(1)} &= \frac{1}{2}h_{mm}\bar{m}^\mu + \frac{1}{2}h_{m\bar{m}}m^\mu - h_{ml}n^\mu - h_{mn}l^\mu.
\end{aligned} \tag{A1}$$

Note that in order to have this explicit form a choice of the first order null directions was made. To relate this to the metric perturbation recall that $g_{\mu\nu} = 2l_{(\mu}n_{\nu)} - 2m_{(\mu}\bar{m}_{\nu)}$ which implies that $h_{\mu\nu} = 2l_{(\mu}^{(1)}n_{\nu)} + 2l_{(\mu}n_{\nu)}^{(1)} - 2m_{(\mu}^{(1)}\bar{m}_{\nu)} - 2m_{(\mu}\bar{m}_{\nu)}^{(1)}$.

Making use of the relations (A1) we can immediately derive the first order Newman-Penrose directional derivatives

$$\begin{aligned}
D^{(1)} &= l^{\mu(1)}\partial_\mu = -\frac{1}{2}h_{ll}\Delta, \\
\Delta^{(1)} &= n^{\mu(1)}\partial_\mu = -\frac{1}{2}h_{nn}D - h_{nl}\Delta, \\
\delta^{(1)} &= m^{\mu(1)}\partial_\mu = \frac{1}{2}h_{mm}\bar{\delta} + \frac{1}{2}h_{m\bar{m}}\delta - h_{ml}\Delta - h_{mn}D.
\end{aligned} \tag{A2}$$

In order to compute the spin coefficients to the required order we follow Ref. [44] making use of the commutation relations [31], Ch. 1.8 (these are exact expressions)

$$\begin{aligned}
\Delta D - D\Delta &= (\gamma + \bar{\gamma})D + (\epsilon + \bar{\epsilon})\Delta - (\bar{\tau} + \pi)\delta - (\tau + \bar{\pi})\bar{\delta}, \\
\delta D - D\delta &= (\bar{\alpha} + \beta - \bar{\pi})D + \kappa\Delta - (\bar{\rho} + \epsilon - \bar{\epsilon})\delta - \sigma\bar{\delta}, \\
\delta\Delta - \Delta\delta &= -\bar{\nu}D + (\tau - \bar{\alpha} - \beta)\Delta + (\mu + \bar{\gamma} - \gamma)\delta - \bar{\lambda}\bar{\delta}, \\
\bar{\delta}\delta - \delta\bar{\delta} &= (\bar{\mu} - \mu)D + (\bar{\rho} - \rho)\Delta + (\alpha - \bar{\beta})\delta + (\beta - \bar{\alpha})\bar{\delta},
\end{aligned} \tag{A3}$$

expanding both sides to first perturbative order and using Eq. (A2) we can equate the coefficients of each operator to get a system of linear equations (16 of which only 12 are independent) that can be solved for the spin coefficients giving

$$\begin{aligned}
k^{(1)} &= (D - \bar{\rho} - 2\epsilon)h_{lm} - \frac{1}{2}(\delta - 2\alpha - 2\beta + \bar{\pi} + \tau)h_{ll}, \\
\sigma^{(1)} &= (\bar{\pi} + \tau)h_{lm} + \frac{1}{2}(D + \rho - \bar{\rho} + 2\bar{\epsilon} - 2\epsilon)h_{mm}, \\
\nu^{(1)} &= -(\Delta + \bar{\mu} + 2\gamma)h_{n\bar{m}} + \frac{1}{2}(\bar{\delta} + 2\alpha + 2\bar{\beta} - \pi - \bar{\tau})h_{nn}, \\
\lambda^{(1)} &= -(\bar{\tau} + \pi)h_{n\bar{m}} - \frac{1}{2}(\Delta + \bar{\mu} - \mu + 2\gamma - 2\bar{\gamma})h_{\bar{m}\bar{m}}, \\
2\mu^{(1)} &= \rho h_{nn} - (\delta + 2\beta + \tau)h_{n\bar{m}} + (\bar{\delta} + 2\bar{\beta} - 2\pi - \bar{\tau})h_{nm} - \frac{1}{2}(2\Delta + \bar{\mu} - \mu + \gamma - \bar{\gamma})h_{m\bar{m}} \\
2\rho^{(1)} &= \bar{\mu}h_{ll} + (\rho - \bar{\rho})h_{nl} + (D + \rho - \bar{\rho})h_{m\bar{m}} - (\delta - 2\bar{\alpha} - \bar{\pi})h_{l\bar{m}} + (\bar{\delta} + 2\bar{\tau} - 2\alpha + \pi)h_{lm}, \\
2\epsilon^{(1)} &= (D + \rho - \bar{\rho})h_{nl} + \frac{1}{2}(\bar{\delta} - 2\alpha - \pi)h_{lm} - \frac{1}{2}(\delta - 2\bar{\alpha} + 3\pi + 4\tau)h_{l\bar{m}} \\
&\quad + \frac{1}{2}(\rho - \bar{\rho})h_{m\bar{m}} - \frac{1}{2}(\Delta + 2\gamma)h_{ll}, \\
2\pi^{(1)} &= -(D - \rho - 2\epsilon)h_{n\bar{m}} - (\bar{\delta} + \bar{\tau} + \pi)h_{nl} - (\Delta + \bar{\mu} - 2\bar{\gamma})h_{l\bar{m}} - \bar{\tau}h_{m\bar{m}} - \tau h_{\bar{m}\bar{m}}, \\
2\tau^{(1)} &= (D - \bar{\rho} + 2\bar{\epsilon})h_{nm} + (\delta - \bar{\pi} - \tau)h_{nl} + (\Delta + \mu - 2\gamma)h_{lm} - \bar{\pi}h_{m\bar{m}} - \pi h_{mm}, \\
2\alpha^{(1)} &= \frac{1}{2}(D - 2\bar{\rho} - \rho - 2\epsilon)h_{n\bar{m}} - \frac{1}{2}(\Delta + 4\gamma - 2\mu + \bar{\mu} - 2\bar{\gamma})h_{l\bar{m}} \\
&\quad - \frac{1}{2}(\bar{\delta} + \pi + \bar{\tau})h_{nl} + \frac{1}{2}(\bar{\delta} + 2\alpha - \pi - \bar{\tau})h_{m\bar{m}} - \frac{1}{2}(\delta - 2\bar{\alpha} + \bar{\pi} + \tau)h_{\bar{m}\bar{m}}, \\
2\beta^{(1)} &= \frac{1}{2}(D - \bar{\rho} - 4\epsilon + 2\rho + 2\bar{\epsilon})h_{nm} - \frac{1}{2}(\Delta + \mu + 2\bar{\mu} + 2\gamma)h_{lm} \\
&\quad - \frac{1}{2}(\delta + \bar{\pi} + \tau)h_{nl} - \frac{1}{2}(\delta - 2\beta + \bar{\pi} + \tau)h_{m\bar{m}} + \frac{1}{2}(\bar{\delta} + 2\beta - \pi - \bar{\tau})h_{mm},
\end{aligned} \tag{A4}$$

$$\begin{aligned}
2\gamma^{(1)} &= -(\bar{\gamma} + \gamma) h_{nl} + \frac{1}{2}(D + \rho - \bar{\rho} + 2\bar{\epsilon}) h_{nn} - \frac{1}{2}(\delta + 2\beta + 2\bar{\pi} + 3\tau) h_{n\bar{m}} \\
&\quad + \frac{1}{2}(\bar{\delta} + 2\bar{\beta} - 2\pi - \bar{\tau}) h_{nm} + \frac{1}{4}(3\bar{\mu} - 2\mu + \gamma - \bar{\gamma}) h_{m\bar{m}}
\end{aligned}$$

Note that these expressions are completely independent of the choice of the gauge, although a tetrad choice to first order had to be made in Eq. (A1).

Finally, the *exact* Weyl scalars are

$$\psi_0 = (D - 3\epsilon + \bar{\epsilon} - \rho - \bar{\rho})\sigma - (\delta - \bar{\alpha} - 3\beta + \bar{\pi} - \tau)\kappa, \quad (\text{A5})$$

$$\psi_1 = (D + \bar{\epsilon} - \bar{\rho})\beta - (\delta - \bar{\alpha} + \bar{\pi})\epsilon - (\alpha + \pi)\sigma + (\gamma + \mu)\kappa,$$

$$\begin{aligned}
\psi_2 &= [(\bar{\delta} - 2\alpha + \bar{\beta} - \pi - \bar{\tau})\beta - (\delta - \bar{\alpha} + \bar{\pi} + \tau)\alpha \\
&\quad + (D + \epsilon + \bar{\epsilon} + \rho - \bar{\rho})\gamma - (\Delta - \bar{\gamma} - \gamma + \bar{\mu} - \mu)\epsilon \\
&\quad + (\bar{\delta} - \alpha + \bar{\beta} - \bar{\tau} - \pi)\tau - (\Delta - \bar{\gamma} - \gamma + \bar{\mu} - \mu)\rho + 2(\nu\kappa - \lambda\sigma)] / 3,
\end{aligned}$$

$$\psi_3 = (\bar{\delta} + \bar{\beta} - \bar{\tau})\gamma - (\Delta - \bar{\gamma} + \bar{\mu})\alpha + (\epsilon + \rho)\nu - (\beta + \tau)\lambda,$$

and

$$\psi_4 = (\bar{\delta} + 3\alpha + \bar{\beta} + \pi - \bar{\tau})\nu - (\Delta - \bar{\gamma} + 3\gamma + \mu + \bar{\mu})\lambda, \quad (\text{A6})$$

Note that these expressions can be trivially expanded to first perturbative order and hold when matter sources are included.

APPENDIX B: SECOND ORDER NEWMAN-PENROSE QUANTITIES

Taking the same first order choice of the tetrad to second order (we can do this because the final aim is to plug this into an invariant object) one obtains

$$\begin{aligned}
l^{\mu(2)} &= -\left[\frac{1}{2}h_{ll}^{(2)} - h_{ll}^{(1)}h_{ln}^{(1)} + 2h_{l\bar{m}}^{(1)}h_{lm}^{(1)}\right] n^\mu, \\
n^{\mu(2)} &= -\left[\frac{1}{2}h_{nn}^{(2)} + 2h_{n\bar{m}}^{(1)}h_{nm}^{(1)}\right] l^\mu - \left[h_{nl}^{(2)} - h_{ll}^{(1)}h_{nn}^{(1)} + \frac{1}{2}\left(h_{lm}^{(1)}h_{n\bar{m}}^{(1)} + h_{l\bar{m}}^{(1)}h_{nm}^{(1)}\right)\right] n^\mu, \\
m^{\mu(2)} &= -\left[h_{mn}^{(2)} + h_{n\bar{m}}^{(1)}h_{mm}^{(1)} + h_{m\bar{m}}^{(1)}h_{nm}^{(1)}\right] l^\mu - \left[h_{ml}^{(2)} + h_{l\bar{m}}^{(1)}h_{mm}^{(1)} + h_{m\bar{m}}^{(1)}h_{lm}^{(1)}\right] n^\mu \\
&\quad + \frac{1}{2}\left[h_{m\bar{m}}^{(2)} + \frac{1}{2}h_{m\bar{m}}^{(1)}h_{mm}^{(1)} + \frac{1}{2}h_{m\bar{m}}^{(1)}h_{m\bar{m}}^{(1)}\right] m^\mu + \frac{1}{2}\left[h_{m\bar{m}}^{(2)} + h_{m\bar{m}}^{(1)}h_{m\bar{m}}^{(1)}\right] \bar{m}^\mu.
\end{aligned} \quad (\text{B1})$$

We now expand up to second order the third commutator of Eq. (A2) to obtain $\nu^{(2)} \doteq \nu_L^{(2)} + \nu_Q^{(2)}$ and $\lambda^{(2)} \doteq \lambda_L^{(2)} + \lambda_Q^{(2)}$

$$\begin{aligned}
\nu_L^{(2)} &= -(\Delta + \bar{\mu} + 2\gamma)h_{n\bar{m}}^{(2)} + \frac{1}{2}(\bar{\delta} + \pi - \bar{\tau})h_{nn}^{(2)}, \\
\nu_Q^{(2)} &= -(\Delta + \bar{\mu} + 2\gamma)h_{nm}^{(1)}h_{m\bar{m}}^{(1)} + 2(\bar{\delta} + \pi - \bar{\tau})h_{nm}^{(1)}h_{n\bar{m}}^{(1)} - \lambda^{(1)}h_{nm}^{(1)} \\
&\quad - \frac{1}{2}\left[(\bar{\delta} + \bar{\tau} - \alpha - \beta)^{(1)} + (\gamma + \bar{\gamma})h_{l\bar{m}}^{(1)}\right] h_{nn}^{(1)} - \left[(\mu - \gamma + \bar{\gamma})^{(1)} - (\gamma + \bar{\gamma})h_{lm}^{(1)}\right] h_{n\bar{m}}^{(1)}, \\
\lambda_L^{(2)} &= -\frac{1}{2}(\Delta + \bar{\mu} - \mu - 2\bar{\gamma} + 2\gamma)h_{m\bar{m}}^{(2)} - (\bar{\tau} + \pi)h_{n\bar{m}}^{(2)}, \\
\lambda_Q^{(2)} &= -\frac{1}{2}(\Delta + \bar{\mu} - \mu - 2\bar{\gamma} + 2\gamma)h_{m\bar{m}}^{(1)}h_{m\bar{m}}^{(1)} + (\bar{\tau} + \pi)\left[h_{m\bar{m}}^{(1)}h_{ln}^{(1)} - h_{m\bar{m}}^{(1)}h_{nm}^{(1)} - \frac{1}{2}h_{m\bar{m}}^{(1)}h_{nn}^{(1)}\right] \\
&\quad - \frac{1}{2}\lambda^{(1)}h_{m\bar{m}}^{(1)} - \frac{1}{2}\left[(\bar{\mu} - \bar{\gamma} + \gamma)^{(1)} - \frac{1}{2}\bar{\rho}h_{nn}^{(1)} + (\mu - \gamma + \bar{\gamma})h_{ln}^{(1)}\right] h_{m\bar{m}}^{(1)}.
\end{aligned} \quad (\text{B2})$$

Finally, using Eq. (A6) we find $\psi_4^{(2)} \doteq \psi_{4L}^{(2)} + \psi_{4Q}^{(2)}$,

$$\begin{aligned}\psi_{4L}^{(2)} &= (\bar{\delta} + 3\alpha + \bar{\beta} + \pi - \bar{\tau})\nu_L^{(2)} - (\Delta + \bar{\mu} + \mu - \bar{\gamma} + 3\gamma)\lambda_L^{(2)}, \\ \psi_{4Q}^{(2)} &= (\bar{\delta} + 3\alpha + \bar{\beta} + \pi - \bar{\tau})\nu_Q^{(2)} - (\Delta + \bar{\mu} + \mu - \bar{\gamma} + 3\gamma)\lambda_Q^{(2)} \\ &\quad + (\bar{\delta} + 3\alpha + \bar{\beta} + \pi - \bar{\tau})^{(1)}\nu^{(1)} - (\Delta + \bar{\mu} + \mu - \bar{\gamma} + 3\gamma)^{(1)}\lambda^{(1)}.\end{aligned}\tag{B3}$$

APPENDIX C: GAUGE INVARIANTS IN THE SCHWARZSCHILD LIMIT

In the case when $a = 0$, we can find the following set of *first* order gauge vectors assuming that the ξ_m^r is given by Eq. (43)

$$\begin{aligned}\xi_m^\vartheta &= -\frac{\cos\vartheta(2h_{\varphi\varphi} + 2\sin^2\vartheta r\xi_m^r - \sin^2\vartheta h_{\vartheta\vartheta}) + \sin\vartheta(2imh_{\vartheta\varphi} - h_{\varphi\varphi,\vartheta} - 2\sin^2\vartheta r\xi_{m,\vartheta}^r)}{2r^2\sin\vartheta(m^2 + 1)}, \\ im\xi_m^t &= \frac{r}{2(r-3M)}\{rh_{t\varphi,r} - 2h_{t\varphi} + r^3\sin^2\vartheta\xi_{m,rt}^\varphi + im(r-2M)\xi_{m,r}^t\} \\ im\xi_m^\varphi &= -\frac{1}{2r^2\sin^2\vartheta(m^2 + 1)}\{(m^2 + 1 - 2\cos^2\vartheta)h_{\varphi\varphi} + \cos^2\vartheta\sin^2\vartheta h_{\vartheta\vartheta} \\ &\quad + \cos\vartheta\sin\vartheta(h_{\varphi\varphi,\vartheta} - 2imh_{\vartheta\varphi} + \sin^2\vartheta r\xi_{m,\vartheta}^r) + 2\sin^2\vartheta(m^2 + \sin^2\vartheta)\xi_m^r\}, \\ \xi_{m,\vartheta}^t &= -\frac{r}{\sin 2\vartheta(r-2M)(r-3M)}\{-imr^2h_{t\varphi,r} + m^2r^2\xi_{m,r}^t - 4m^2Mr\xi_{m,r}^t - imr^4\sin^2\vartheta\xi_{m,tr}^\varphi \\ &\quad + 2imMrh_{t\varphi,r} + 4m^2M^2\xi_{m,r}^t + 2imMR^3\sin^2\vartheta\xi_{m,tr}^\varphi + 2imMh_{t\varphi} - 6Mr\sin^2\vartheta\xi_{m,t}^r + 2r^2\sin^2\vartheta\xi_{m,t}^r \\ &\quad - \sin 2\vartheta(3Mh_{t\vartheta} - rh_{t\vartheta}) - 3Mh_{\varphi\varphi,t} + rh_{\varphi\varphi,t}r\}\end{aligned}\tag{C1}$$

$$\begin{aligned}\xi_{m,\vartheta}^\varphi &= -\frac{i}{(2r^2(m^2 + 1)\sin^3\vartheta)}\left(-2i\sin\vartheta\cos^2\vartheta h_{\vartheta\varphi} + 2m\cos\vartheta h_{\varphi\varphi} + 2m\cos\vartheta\sin^2\vartheta r\xi_m^r \right. \\ &\quad \left. - 2ih_{\vartheta\varphi}\sin^3\vartheta - m\sin^2\vartheta\cos\vartheta h_{\vartheta\vartheta} - m\sin\vartheta h_{\varphi\varphi,\vartheta} - 2m\sin^3\vartheta r\xi_{m,\vartheta}^r\right), \\ \xi_{m,t}^t &= -\frac{2Mr^2\xi_m^r + h_{tt}}{2r(r-2M)} \\ \xi_{m,t}^\varphi &= -\frac{(r-2M)[rh_{t\varphi,r} + r^3\sin^2\vartheta\xi_{m,rt}^\varphi + im(r-2M)\xi_{m,r}^t] - 2Mh_{t\varphi}}{2r^2\sin^2\vartheta(r-3M)}\end{aligned}\tag{C2}$$

$\xi_{,r}^\varphi$ and $\xi_{,r}^t$ as given by Eqs. (46) and (45) are well defined in the $a \rightarrow 0$ limit.

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