

Worldtube puncture scheme for first- and second-order self-force calculations in the Fourier domain

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Second-order gravitational self-force theory has recently led to the breakthrough calculation of “first post-adiabatic” (1PA) compact-binary waveforms [Phys. Rev. Lett. 130, 241402 (2023)]. The computations underlying those waveforms depend on a method of solving the perturbative second-order Einstein equation on a Schwarzschild background in the Fourier domain. In this paper we present that method, which involves dividing the domain into several regions. Different regions utilize different time slicings and allow for the use of “punctures” to tame sources and enforce physical boundary conditions. We demonstrate the method for Lorenz-gauge and Teukolsky equations in the relatively simple case of calculating parametric derivatives (“slow time derivatives”) of first-order fields, which are an essential input at second order.

I. INTRODUCTION

A. Waveform generation and second-order self-force theory

In recent years, gravitational self-force theory [1, 2] has reached a mature stage of producing practical models of compact-binary waveforms [3–7]. These models, targeted at asymmetric binaries in which one body is much more massive than the other, have traditionally been motivated by the need to model waveforms from extreme-mass-ratio inspirals (EMRIs) with mass ratios $\varepsilon := \mu/M \sim 10^{-5}$ [8], where M is the mass of the larger body, and μ is the mass of the companion. However, the resulting waveforms have proved to be quite accurate even for mass ratios $\sim 10^{-1}$ [7].

The method underlying these models is an expansion of the spacetime metric in powers of ε , with the assumption that the zeroth-order spacetime is a stationary black hole. From that starting point, a combination of perturbative techniques are used, including broad strategies adapted from singular perturbation theory (matched asymptotic expansions, multiscale expansions, and related methods) as well as the specific tools of black hole perturbation theory [1, 2].

Most of this progress in waveform modeling has been driven by calculations in the Fourier domain [2–7, 9, 10]. While there has been continued progress in time-domain calculations [11–14], and while it is possible to construct practical surrogate models [15] from a bank of time-domain waveforms, most development has been on Fourier methods that leverage the disparate time scales in small-mass-ratio binaries: the fast orbital time scale $\sim M$ and the slow time scale $\sim M/\varepsilon$ over which the system evolves. This separation of scales allows one to divide waveform generation into two steps: an expensive offline step in which one solves Fourier-domain field equa-

tions on a grid of slowly evolving parameter values (e.g., eccentricity, semi-latus rectum, the mass and spin of the primary black hole, etc.); and a fast, cheap online step of solving simple ordinary differential equations (ODEs) to evolve through the parameter space. The flexibility and efficiency of such a framework is exemplified by the **Fast EMRI Waveforms** package [3].

This method can be carried to any order in ε by using a multiscale expansion of the Einstein equations [2, 9], which builds on the multiscale form of the companion’s orbital motion around the primary [16]. Orbits around a Kerr black hole generically have three slowly evolving frequencies $\Omega_A = (\Omega_r, \Omega_\theta, \Omega_\phi)$ corresponding to azimuthal motion (Ω_ϕ), orbital precession associated with eccentricity (Ω_r), and precession of the orbital plane around the primary’s spin axis (Ω_θ). Any given (ℓ, m) multipole of the resulting waveform then takes the simple form [2]

$$h_{\ell m} = \sum_{k^i} \left[\varepsilon h_{\ell m}^{(1, k^i)}(\mathcal{J}_I) + \varepsilon^2 h_{\ell m}^{(2, k^i)}(\mathcal{J}_I) + \dots \right] e^{-i(m\varphi_\phi + k^i\varphi_i)}, \quad (1)$$

where $k^i = (k^r, k^\theta)$ are integers running from $-\infty$ to $+\infty$, \mathcal{J}_I are the binary’s slowly evolving parameters, and $\varphi_A = (\varphi_r, \varphi_\theta, \varphi_\phi)$ are the orbital phases associated with the three frequencies Ω_A . The time dependence of the waveform is governed by simple ODEs of the form

$$\frac{d\varphi_A}{du} = \Omega_A(\mathcal{J}_I), \quad (2)$$

$$\frac{d\mathcal{J}_I}{du} = \varepsilon[F_I^{(0)}(\mathcal{J}_K) + \varepsilon F_I^{(1)}(\mathcal{J}_K) + \dots], \quad (3)$$

where u denotes retarded time at future null infinity. The slowly evolving amplitudes $h_{\ell m}^{(n, k^i)}$, frequencies Ω_A , and driving forces $F_I^{(n)}$ are pre-computed in the offline step, and the waveform is then rapidly generated by solving the ODEs (2) and (3).

A model that uses only the leading forcing term $F_I^{(0)}$ is referred to as adiabatic (“OPA”); this requires solving the linearized Einstein or Teukolsky equation in the offline step. A model that includes terms up to and including $F_I^{(n)}$ is referred to as n th post-adiabatic (n PA); this requires solving the Einstein equations through order ε^{n+1} . In the offline step, the Einstein equations are formulated in a discrete Fourier domain based on mode expansions in the orbital phases φ_A , as displayed in Eq. (1).

The most advanced self-force calculations use this multiscale method to solve the Einstein equations through second order in ε [7, 17, 18], yielding 1PA waveforms [7]. Those calculations are currently restricted to the simplest scenario of quasicircular inspirals into Schwarzschild black holes, in which case the problem simplifies because (i) there is only one orbital frequency (Ω_ϕ) and its associated azimuthal phase, and (ii) the perturbative Einstein equations on the Schwarzschild background are fully separable.

In Ref. [9], we presented the multiscale Einstein equations for this special case of quasicircular, nonspinning binaries. In this paper, we present a method of solving such equations: a worldtube puncture scheme in the Fourier domain. This scheme, which builds on earlier work by Warburton and Wardell [19, 20], was a key tool in the second-order calculations in Refs. [7, 17, 18]. It extends Refs. [19, 20] by allowing for noncompact sources, irregular boundary conditions, and arbitrary choices of time variable. Its main new ingredients are subtractions of punctures in multiple regions and differing choices of time slicing in different regions.

Punctures have traditionally been used because self-force calculations work by “skeletonizing” the small companion, reducing it to a point-particle singularity. In that context, puncture schemes subtract off the dominant, singular part of the particle’s gravitational field in a worldtube surrounding the particle and then solve a field equation for the regular residual piece. First presented in practical forms in Refs. [21, 22], these schemes are now a standard method in self-force theory [1, 2, 23]; most pertinently, they have underpinned most descriptions of second-order self-force theory [24–28]. Our scheme leans even more heavily on this puncture method by introducing additional punctures at the black hole horizon and at infinity.

Use of alternative slicings in Fourier-domain self-force calculations is a more recent development. The multiscale field equations in Ref. [9], which were the basis for the calculations in Refs. [7, 17, 18], were formulated using a hyperboloidal time variable¹. Slices of constant hyperboloidal time penetrate the future horizon of the primary black hole and extend to future null infinity

rather than to spatial infinity, as illustrated in Fig. 1. This has key advantages in a multiscale expansion, significantly improving the behaviour of the source terms in the second-order field equations, reducing the need to derive punctures, and simplifying waveform extraction. More recently, Ref. [29] extended this approach by compactifying the hyperboloidal surfaces and working with a spectral method. Those modifications bring additional advantages and are part of a longer-term introduction of hyperboloidal methods into black hole perturbation theory [30–32]. Here, for historical reasons, we do not adopt these additional tools, but we delineate the relative merits of each method. We are also careful to note that compactified hyperboloidal slices do not evade the fundamental breakdown of the multiscale expansion at large distances; this breakdown, which was explored in Ref. [33], has necessitated the use of an alternative, post-Minkowski expansion at large distances in current second-order self-force calculations. Details of that expansion will be presented elsewhere.

B. Outline and conventions

We begin in Sec. II by reviewing the multiscale expansion of the Einstein field equations. This review broadly follows Ref. [9]’s treatment of quasicircular inspirals into Schwarzschild black holes, but we take the opportunity to present that treatment in a more geometrical form that is not tied to the Lorenz gauge or to a tensor-harmonic decomposition. We also discuss how it straightforwardly extends to the case of eccentric orbits.

In Secs. III and IV we summarize two specific forms of the multiscale equations. Section III summarizes the Lorenz-gauge field equations, again following Ref. [9]. Here we decompose the multiscale metric perturbation into tensor spherical harmonics, reducing the field equations to a radial ODE for each mode. Since our worldtube scheme is quite generic, in Sec. IV we also present the Teukolsky equation in this multiscale framework, building on recent work in Refs. [34] and [35].

Sections V–VIII then present our worldtube puncture scheme in a generic form applicable to both the Lorenz-gauge and Teukolsky equations. The method of solving the equations is based on variation of parameters. We consider various formulations of that method and its application to the various types of field equations that arise.

In Secs. IX and X, we demonstrate the method in the Lorenz-gauge and Teukolsky versions. The demonstrations consist of solving a field equation for a parametric derivative (a derivative with respect to orbital radius) of the first-order-in- ε field (the metric perturbation in the Lorenz-gauge case and the Weyl scalar in the Teukolsky case). Such parametric derivatives are important in the multiscale expansion because they enter into the source terms in the second-order field equations. In the case of Lorenz-gauge perturbations, we find agreement with results for the same quantity as calculated using a different

¹ We use the term “hyperboloidal” loosely. In the standard definition, hyperboloidal slices are required to be everywhere spacelike in the black hole’s exterior, while we allow for slices containing null segments.

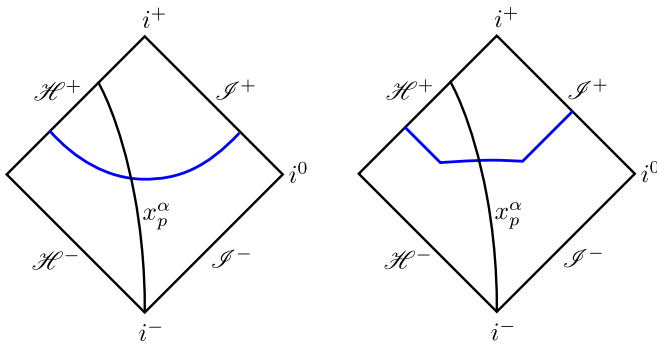


FIG. 1. Penrose diagrams of the Schwarzschild exterior illustrating a particle's trajectory x_p^α along with slices (blue curves) of constant hyperboloidal time $s = t - k(r^*)$. s transitions from advanced time $v = t + r^*$ near the future horizon to retarded time $u = t - r^*$ near future null infinity. Left: a smooth choice of slicing (which may or may not be everywhere spacelike in the Schwarzschild exterior). Right: sharp slicing in which $s = v$ in a region to the left of the particle, $s = t$ in a region containing the particle, and $s = u$ in a region to the right of the particle.

method in Ref. [36].

Finally, in the concluding section, Sec. XI, we discuss the relative merits of our variation-of-parameters approach versus the more recent alternatives in Refs. [36] and [29].

Throughout the paper we use a mostly positive metric signature, $(-, +, +, +)$, and geometrical units with $G = c = 1$. Indices are raised and lowered with the background Schwarzschild metric $g_{\alpha\beta}$, and ∇ and a semicolon both denote the covariant derivative compatible with $g_{\alpha\beta}$. (t, r, θ, ϕ) denote Schwarzschild coordinates, in which $g_{\alpha\beta} = \text{diag}(-f, f^{-1}, r^2, r^2 \sin^2 \theta)$, where $f := 1 - 2M/r$.

II. EINSTEIN FIELD EQUATIONS IN MULTISCALE FORM

In this section we review the perturbative Einstein field equations for a binary with a small mass ratio ε . We first explain the expansion as formulated in regular perturbation theory and then explain how we formulate it in our multiscale form. We particularly highlight (i) the role of spacetime foliations, (ii) the discrete Fourier expansion of the field equations, and (iii) the appearance of parametric derivatives as source terms. We refer to Refs. [2, 9] for more details. Our formulation here is a more geometrical form of the expansion described in Appendix A of Ref. [9].

A. Regular perturbation theory

In regular perturbation theory, we expand the exact metric $\mathbf{g}_{\mu\nu}$ and stress-energy tensor $T_{\mu\nu}$ as

$$\mathbf{g}_{\mu\nu}(y, \varepsilon) = g_{\mu\nu}(y) + \varepsilon h_{\mu\nu}^{(1)}(y) + \varepsilon^2 h_{\mu\nu}^{(2)}(y) + O(\varepsilon^3) \quad (4)$$

and

$$T_{\mu\nu}(y, \varepsilon) = \varepsilon T_{\mu\nu}^{(1)}(y) + \varepsilon^2 T_{\mu\nu}^{(2)}(y) + O(\varepsilon^3), \quad (5)$$

where y stands for some coordinates y^μ . At least through second order in ε , $T_{\mu\nu}$ can be taken to be the Detweiler stress-energy tensor [25, 37],²

$$T_{\mu\nu} = \mu \int \tilde{u}_\mu \tilde{u}_\nu \frac{\delta^4(y - y_p)}{\sqrt{-\tilde{g}}} d\tilde{\tau}, \quad (6)$$

where μ is the mass of the particle, y_p^μ is its worldline, $\tilde{u}_\mu := \tilde{g}_{\mu\alpha} \frac{dy_p^\alpha}{d\tilde{\tau}}$, $\tilde{g}_{\mu\nu}$ is a certain effective metric of the form

$$\tilde{g}_{\mu\nu}(y, \varepsilon) = g_{\mu\nu}(y) + \varepsilon h_{\mu\nu}^{\text{R}(1)}(y) + \varepsilon^2 h_{\mu\nu}^{\text{R}(2)}(y) + O(\varepsilon^3), \quad (7)$$

$\tilde{\tau}$ is the proper time in that metric, and $h_{\mu\nu}^{\text{R}(n)}$ are certain smooth vacuum perturbations extracted from $h_{\mu\nu}^{(n)}$. The worldline y_p^μ obeys the geodesic equation in $\tilde{g}_{\mu\nu}$ or an equivalent self-forced equation of motion in $g_{\mu\nu}$ [26, 42].

Given these expansions, the Einstein equation $G_{\mu\nu}[g] = 8\pi T_{\mu\nu}$ becomes a hierarchical sequence of equations, the first three of which are

$$G_{\mu\nu}[g] = 0, \quad (8)$$

$$G_{\mu\nu}^{(1)}[h^{(1)}] = 8\pi T_{\mu\nu}^{(1)}, \quad (9)$$

$$G_{\mu\nu}^{(1)}[h^{(2)}] = 8\pi T_{\mu\nu}^{(2)} - G_{\mu\nu}^{(2)}[h^{(1)}, h^{(1)}]. \quad (10)$$

Here $G_{\mu\nu}^{(1)}[h]$ is the linearized Einstein tensor constructed from a perturbation $h_{\mu\nu}$, and $G_{\mu\nu}^{(2)}[h, h]$ is the quadratic

² We note that because of the strongly divergent fields at second order, the stress-energy tensor (6) and field equation (10) have only been derived in a class of “highly regular” gauges and in gauges smoothly related to Lorenz [37]. In the Lorenz-gauge case, the derivation requires adopting a certain canonical distributional definition of $G_{\mu\nu}^{(2)}[h^{(1)}, h^{(1)}]$. We will not concretely require that definition here, but we return to this point in the Conclusion, Sec. XI. However, we also note that no concrete second-order calculations have directly used Eq. (10) but instead have used a puncture scheme, which is a more primitive formulation that does not involve these subtleties. We write the field equations here in terms of a stress-energy tensor only to simplify the presentation. Like the stress-energy tensor, concrete punctures are only available in highly regular and smoothly deformed Lorenz gauges [38, 39], but this does not restrict the choice of gauge when solving the field equations: independent of the puncture's gauge, the numerical variable (the residual field) can be in any convenient gauge; see, for example, Refs. [40, 41].

term in the expansion of the Einstein tensor. We write $G_{\mu\nu}^{(1)}[h]$ as

$$G_{\mu\nu}^{(1)}[h] = -\frac{1}{2}E_{\mu\nu}[\bar{h}] + \nabla_{(\mu}Z_{\nu)}[\bar{h}] - \frac{1}{2}g_{\mu\nu}\nabla_{\alpha}Z^{\alpha}[\bar{h}], \quad (11)$$

in terms of the trace-reversed field

$$\bar{h}_{\mu\nu} := h_{\mu\nu} - \frac{1}{2}g_{\mu\nu}g^{\alpha\beta}h_{\alpha\beta} \quad (12)$$

and the linear operators

$$E_{\alpha\beta}[\bar{h}] := \square\bar{h}_{\alpha\beta} + 2R_{\alpha}{}^{\mu}{}_{\beta}{}^{\nu}\bar{h}_{\mu\nu}, \quad (13)$$

$$Z_{\alpha}[\bar{h}] := g^{\beta\gamma}\nabla_{\gamma}\bar{h}_{\alpha\beta}, \quad (14)$$

with $\square := g^{\mu\nu}\nabla_{\mu}\nabla_{\nu}$. The quadratic Einstein tensor $G_{\mu\nu}^{(2)}[h, h]$ is written explicitly in Eq. (4) of Ref. [2], but we will not need its explicit form here.

Given the background metric $g_{\mu\nu}$, regular perturbation theory reduces to solving the sequence of linear field equations (9), (10), and so on to higher order.

B. Multiscale expansion

The multiscale expansion of the field equations differs in important ways from a regular expansion. It is designed to maintain uniform accuracy while capturing the binary’s “fast” evolution on the time scale $\sim M$, due to the orbiting particle, and the “slow” evolution on the time scale $\sim M/\varepsilon$, due to dissipation.

The method begins with a choice of time function, which we write as

$$s = s(t, r) := t - k(r^*). \quad (15)$$

Here r^* is the standard tortoise coordinate, $r^* = r + 2M \ln[r/(2M) - 1]$, and $k(r^*)$ is a height function. We choose $k(r^*)$ such that

$$k(r^*) \rightarrow +r^* \quad \text{for } r^* \rightarrow \infty, \quad (16)$$

$$k(r^*) \rightarrow -r^* \quad \text{for } r^* \rightarrow -\infty. \quad (17)$$

This ensures that slices of constant s are hyperboloidal, by which we mean they reduce to surfaces of constant advanced time $v = t + r^*$ at the future horizon (\mathcal{H}^+) and to surfaces of constant retarded time $u = t - r^*$ at future null infinity (\mathcal{I}^+), as illustrated in Fig. 1. With our loose definition of the term “hyperboloidal”, we do not require these slices to be everywhere spacelike in the Schwarzschild exterior, nor do we require them to be smooth.

For most of this paper, we leave s unspecified. However, we mention here our preferred, “sharp” foliation used in our numerical calculations. This slicing, illustrated in the right panel of Fig. 1, uses a piecewise height function,

$$k(r^*) = \begin{cases} -r^* & \text{for } r < r_1, \\ 0 & \text{for } r_1 < r < r_2, \\ +r^* & \text{for } r > r_2, \end{cases} \quad (18)$$

where r_1 (r_2) is a radius smaller (larger) than the particle’s orbital radius. With this choice, $s = v$ in a region extending to \mathcal{H}^+ ; $s = t$ in a region containing the particle; and $s = u$ in a region extending to \mathcal{I}^+ . We will refer to this as v - t - u slicing. It provides a simple way of avoiding steep gradients within a numerical domain. The sharp change in slicing will cause finite differentiability or jumps in various fields when crossing r_1 and r_2 , but these effects are easily controlled. The switching points are placed at boundaries between domains, and the sharp change in slicing is accounted for using easily derived junction conditions at these domain boundaries (a familiar procedure from dealing with point-particle sources in radial differential equations).

Given a choice of time function s , we assume that the metric’s dependence on s is fully encoded in a dependence on the binary’s mechanical variables.³ For the quasicircular inspirals we focus on here, the time-dependent mechanical variables are (i) the particle’s orbital phase ϕ_p , (ii) its orbital frequency $\Omega := d\phi_p/ds$, and (iii) corrections to the central black hole’s mass and spin, $\varepsilon\delta M_A = (\varepsilon\delta M, \varepsilon\delta J)$ (with the overall factor of ε pulled out to make δM_A order unity). The spacetime’s slow evolution is encoded in the metric’s dependence on the parameters $\mathcal{J}_I = (\Omega, \delta M_A)$, which evolve due to the dissipative self-force (in the case of Ω) or due to fluxes through the horizon (in the case of δM_A). The evolution on the fast orbital time scale $\sim 1/\Omega$ is encoded in a periodic dependence on the orbital phase ϕ_p . We comment below on how this extends to the case of eccentric orbits.

More concretely, for quasicircular orbits the system’s evolution is governed by the rates of change of ϕ_p and \mathcal{J}_I . We expand those rates of change in powers of ε at fixed phase-space coordinate values (ϕ_p, \mathcal{J}_I) :

$$\dot{\phi}_p = \Omega, \quad (19)$$

$$\dot{\Omega} = \varepsilon \left[F_{\Omega}^{(0)}(\Omega) + \varepsilon F_{\Omega}^{(1)}(\Omega, \delta M_A) + \mathcal{O}(\varepsilon^2) \right], \quad (20)$$

$$\delta \dot{M}_A = \varepsilon \left[F_A^{(0)}(\Omega) + \varepsilon F_A^{(1)}(\Omega, \delta M_B) + \mathcal{O}(\varepsilon^2) \right], \quad (21)$$

where a dot denotes d/ds [cf. Eqs. (2)–(3)]. In these expansions, the numerical labels denote the post-adiabatic

³ This means that we exclude a variety of effects, including gauges that do not conform to our assumed multiscale time dependence. For example, we exclude gauges that blow up with time and incoming gauge modes that could be sent into the system with arbitrary frequencies. In the case of eccentric orbits, our assumptions also fail at $r - \phi$ resonant kicks [43], though that effect is higher order than we consider here. Hereditary effects associated with gravitational-wave memory (which enter into the multiscale solution at 2PA order through physical boundary conditions at large r [33, 44]) also introduce a type of integrated dependence on the past history of the mechanical variables, as in post-Newtonian theory [45]. However, these hereditary effects are determined by the “current” state of the system’s slowly evolving variables, meaning they do not spoil our assumptions [44].

order at which the quantity enters⁴. The driving forces $F_\Omega^{(n)}$, whose explicit forms are not needed here, are given in terms of the gravitational self-force in Eqs. (A9)–(A10) of Ref. [9], and $F_A^{(0)}(\Omega)$ are the standard leading-order fluxes of energy and angular momentum into the black hole due to an orbiting particle [2, 9]. The particle's orbital trajectory x_p^i in Schwarzschild spatial coordinates $x^i = (r, \theta, \phi)$ takes the simple form

$$x_p^i(\phi_p, \Omega, \varepsilon) = [r_p(\Omega, \varepsilon), \pi/2, \phi_p], \quad (22)$$

where

$$r_p(\Omega, \varepsilon) = r_0(\Omega) + \varepsilon r_1(\Omega) + O(\varepsilon^2). \quad (23)$$

The leading coefficient $r_0 = M(M\Omega)^{-2/3}$ is the standard geodesic relationship; the subleading coefficient, which will not be explicitly needed here, is given in Eq. (A8) of Ref. [9].

In line with our assumption that the spacetime only depends on s through a dependence on (ϕ_p, \mathcal{J}_I) , we now treat the metric as a function on an extended manifold that includes the binary's mechanical phase space. Instead of using the regular expansions (4) and (5), in which we would expand in powers of ε at fixed values of spacetime coordinates (s, x^i) , we now expand the metric and the stress-energy tensor in powers of ε at fixed $(x^i, \phi_p, \mathcal{J}_I)$:

$$\mathbf{g}_{\mu\nu}(x^i, \phi_p, \mathcal{J}_I, \varepsilon) = g_{\mu\nu}(x^i) + \varepsilon h_{\mu\nu}^{(1)}(x^i, \phi_p, \mathcal{J}_I) + \varepsilon^2 h_{\mu\nu}^{(2)}(x^i, \phi_p, \mathcal{J}_I) + O(\varepsilon^3), \quad (24)$$

and

$$T_{\mu\nu}(x^i, \phi_p, \mathcal{J}_I, \varepsilon) = \varepsilon T_{\mu\nu}^{(1)}(x^i, \phi_p, \Omega) + \varepsilon^2 T_{\mu\nu}^{(2)}(x^i, \phi_p, \mathcal{J}_I) + O(\varepsilon^3). \quad (25)$$

The expansion of $T_{\mu\nu}$ is obtained by substituting the multiscale expansions of x_p^i and $\tilde{g}_{\mu\nu}$ into Eq. (6);⁵ in turn, $\tilde{g}_{\mu\nu}$ (along with the punctures and residual fields we introduce later) inherits the multiscale structure of $\mathbf{g}_{\mu\nu}$ as described in Ref. [9]. Each term in these expansions is assumed to be a 2π -periodic function of ϕ_p . The physical metric on spacetime is obtained once the s dependence of ϕ_p and \mathcal{J}_I is determined via Eqs. (19)–(21). Prior to

that determination, we treat $(x^i, \phi_p, \mathcal{J}_I)$ as independent variables.

Substituting the expansions (24) and (25) into the Einstein equations, we obtain a modified version of Eqs. (9)–(10),

$$G_{\mu\nu}^{(1,0)}[h^{(1)}] = 8\pi T_{\mu\nu}^{(1)}, \quad (26)$$

$$G_{\mu\nu}^{(1,0)}[h^{(2)}] = 8\pi T_{\mu\nu}^{(2)} - G_{\mu\nu}^{(2,0)}[h^{(1)}, h^{(1)}] - G_{\mu\nu}^{(1,1)}[h^{(1)}]. \quad (27)$$

The operators $G_{\mu\nu}^{(n,j)}$ act on functions of $(x^i, \phi_p, \mathcal{J}_I)$. They are derived from $G_{\mu\nu}^{(n)}$ using the chain rule

$$\frac{\partial}{\partial y^\alpha} = e_\alpha^i \frac{\partial}{\partial x^i} + s_\alpha \left(\frac{d\phi_p}{ds} \frac{\partial}{\partial \phi_p} + \frac{d\mathcal{J}_I}{ds} \frac{\partial}{\partial \mathcal{J}_I} \right), \quad (28)$$

where

$$e_\alpha^i := \frac{\partial x^i}{\partial y^\alpha} \quad \text{and} \quad s_\alpha := \frac{\partial s}{\partial y^\alpha} \quad (29)$$

are a basis of one-forms. s^α is normal to surfaces of constant s . If $x^i = (r, \theta, \phi)$, then $e_\alpha^r s^\alpha = -dk/dr^*$ and $e_\alpha^i s^\alpha = 0$ for $i = \theta$ or ϕ . Note that in the simple case $y^\alpha = (s, x^i)$, e_α^i and s_α reduce to δ_α^i and δ_α^s , but here we leave y^α generic.

Given Eqs. (19)–(21), the chain rule (28) implies the expansion

$$\nabla_\alpha = \nabla_\alpha^{(0)} + \varepsilon s_\alpha \vec{\partial}_\nu + \mathcal{O}(\varepsilon^2), \quad (30)$$

where the zeroth-order covariant derivative is

$$\nabla_\alpha^{(0)} = e_\alpha^i \frac{\partial}{\partial x^i} + s_\alpha \Omega \frac{\partial}{\partial \phi_p} + \text{Christoffel terms}, \quad (31)$$

$\mathcal{V}_I = (F_\Omega^{(0)}, F_A^{(0)})$ is the leading-order velocity through parameter space, and

$$\vec{\partial}_\nu := \mathcal{V}_I \frac{\partial}{\partial \mathcal{J}_I} = F_\Omega^{(0)} \frac{\partial}{\partial \Omega} + F_A^{(0)} \frac{\partial}{\partial \delta M_A} \quad (32)$$

is a directional derivative in the parameter space.

Using the above expansion of the covariant derivative, we see that $G_{\mu\nu}^{(n,0)}$ is given by $G_{\mu\nu}^{(n)}$ with $\nabla_\alpha \rightarrow \nabla_\alpha^{(0)}$. $G_{\mu\nu}^{(n,1)}$ is given by the terms in $G_{\mu\nu}^{(n)}$ that are linear in the velocity \mathcal{V}_I . Explicitly, the operator that appears at 1PA order is

$$G_{\mu\nu}^{(1,1)}[h] = -\frac{1}{2} E_{\mu\nu}^{(1)}[\bar{h}] + \nabla_{(\mu}^{(0)} Z_{\nu)}^{(1)}[\bar{h}] + \nabla_{(\mu}^{(1)} Z_{\nu)}^{(0)}[\bar{h}] - \frac{1}{2} g_{\mu\nu} \left(\nabla_\alpha^{(0)} Z_{(1)}^\alpha[\bar{h}] + \nabla_\alpha^{(1)} Z_{(0)}^\alpha[\bar{h}] \right). \quad (33)$$

The individual terms in this expression are

$$E_{\mu\nu}^{(1)}[\bar{h}] = s_\alpha s^\alpha F_\Omega^{(0)} \partial_{\phi_p} \bar{h}_{\mu\nu} + 2s^\alpha \nabla_\alpha^{(0)} \left(\vec{\partial}_\nu \bar{h}_{\mu\nu} \right) + \left(\nabla_\alpha^{(0)} s^\alpha \right) \vec{\partial}_\nu \bar{h}_{\mu\nu}, \quad (34)$$

$$Z_\mu^{(1)}[\bar{h}] = s^\alpha \vec{\partial}_\nu \bar{h}_{\mu\alpha}, \quad (35)$$

$$\nabla_\mu^{(1)} Z_\nu^{(0)}[\bar{h}] = s_\mu \vec{\partial}_\nu Z_\nu^{(0)}[\bar{h}]. \quad (36)$$

⁴ This statement assumes that we calculate $F_\Omega^{(n)}$ from energy fluxes to infinity and into the horizon, using a balance law, meaning the leading-order horizon flux $F_A^{(0)}(\Omega)$ enters at 0PA order, and the first subleading horizon flux enters at 1PA order. If $F_\Omega^{(n)}$ is instead calculated using the local self-force, then $F_A^{(0)}(\Omega)$ does not enter until 1PA order. δM_A itself only enters at 1PA order in either approach.

⁵ We note that Eq. (6) is derived within a self-consistent expansion [46] that is more general than either regular perturbation theory or our multiscale expansion.

The contractions involving s_α evaluate to

$$\begin{aligned} s_\alpha s^\alpha &= -f^{-1}(1 - H^2), \\ \nabla_\alpha^{(0)} s^\alpha &= -\frac{dH}{dr} - \frac{2H}{r}, \\ s^\alpha \nabla_\alpha^{(0)} &= -f^{-1}(1 - H^2)\Omega\partial_{\phi_p} - H\partial_r \\ &\quad + \text{Christoffel terms}, \end{aligned} \quad (37)$$

where

$$H := \frac{dk}{dr^*}. \quad (40)$$

These equations simplify significantly if $s = v$ (meaning $H = -1$), $s = t$ (meaning $H = 0$), or $s = u$ (meaning $H = 1$). We repeatedly return to those special cases in later sections.

For any choice of s , the field equations (26)–(27) reduce to partial differential equations in (x^i, ϕ_p) . These can be solved at fixed values of \mathcal{J}_I because derivatives with respect to \mathcal{J}_I only appear as sources, in the term $G_{\mu\nu}^{(1,1)}[h^{(1)}]$.

C. Fourier expansion

Since all functions of ϕ_p are periodic, we can expand them in Fourier series:

$$h_{\alpha\beta}^{(n)}(x^i, \phi_p, \mathcal{J}_I) = \sum_{m=-\infty}^{\infty} h_{\alpha\beta}^{(n,m)}(x^i, \mathcal{J}_I) e^{-im\phi_p}, \quad (41)$$

$$T_{\alpha\beta}^{(n)}(x^i, \phi_p, \mathcal{J}_I) = \sum_{m=-\infty}^{\infty} T_{\alpha\beta}^{(n,m)}(x^i, \mathcal{J}_I) e^{-im\phi_p}. \quad (42)$$

We then have $\frac{\partial}{\partial\phi_p} \rightarrow -im$ when acting on individual modes, implying

$$\nabla_\alpha^{(0)} \rightarrow e_\alpha^i \frac{\partial}{\partial x^i} - is_\alpha \omega_m + \text{Christoffel terms}, \quad (43)$$

where $\omega_m := m\Omega$.

By substituting this Fourier expansion into the field equations (26)–(27), we obtain decoupled differential equations in x^i for each mode $h_{\alpha\beta}^{(n,m)}(x^i, \mathcal{J}_I)$. Again, these can be solved at fixed values of \mathcal{J}_I . As summarized around Eqs. (1)–(3), the waveform-generation scheme used in Ref. [7] then consists of (i) computing and storing the waveform amplitudes $\lim_{r \rightarrow \infty} r h_{\alpha\beta}^{(n,m)}$ and the driving forces $F_I^{(n)}$ on a grid of Ω values, (ii) solving Eqs. (19)–(21) to generate a trajectory through phase space, and (iii) substituting the trajectory into $\lim_{r \rightarrow \infty} \sum_m r h_{\alpha\beta}^{(n,m)}[\mathcal{J}_I(s)] e^{-im\phi_p(s)}$ to obtain the waveform.

Before proceeding, we stress that the discrete Fourier series (41) is *not* a Fourier transform in time. It would only be a Fourier transform if \mathcal{J}_I were independent of s

and if $\phi_p(s)$ were equal to Ωs (with constant Ω). Neither of these conditions hold true for the inspiraling system. Therefore, we are careful to refer to the resulting field equations as being in the Fourier domain but not being in the frequency domain. However, readers familiar with frequency-domain equations can apply virtually all their knowledge directly to our Fourier-domain equations: the left-hand side of the field equation for a mode coefficient $h_{\alpha\beta}^{(n,m)}(x^i, \mathcal{J}_I)$ is identical to the left-hand side of the field equation for the mode coefficient in a frequency-domain expansion $h_{\alpha\beta}^{(n,\omega)}(x^i) e^{-i\omega s}$ (with $\omega = \omega_m$).

We also note that the above description extends, with only minor changes, to the case of eccentric orbits in Schwarzschild. In that case there are two orbital phases, $\varphi_A = (\varphi_r, \varphi_\phi)$, and associated frequencies $\Omega_A = (\Omega_r, \Omega_\phi)$. The Fourier expansion (41) becomes $\sum_{m,k} h_{\alpha\beta}^{(n,m,k)}(x^i, \mathcal{J}_I) e^{-im\varphi_\phi - ik\varphi_r}$ [cf. the expansion (1) in Kerr spacetime]. The adiabatically evolving parameters become $\mathcal{J}_I = (p_i, \delta M_A)$, for example, where $p_i = (p, e)$ are the semilatus rectum and eccentricity. The chain rule (28) becomes

$$\frac{\partial}{\partial y^\alpha} = e_\alpha^i \frac{\partial}{\partial x^i} + s_\alpha \left(\frac{d\varphi_A}{ds} \frac{\partial}{\partial \varphi_A} + \frac{d\mathcal{J}_I}{ds} \frac{\partial}{\partial \mathcal{J}_I} \right), \quad (44)$$

meaning we make the following replacements: $\mathcal{V}_I \rightarrow (F_i^{(0)}, F_A^{(0)})$ and the corresponding adjustment

$$\vec{\partial}_\mathcal{V} \rightarrow F_i^{(0)} \frac{\partial}{\partial p^i} + F_A^{(0)} \frac{\partial}{\partial \delta M_A}; \quad (45)$$

$\Omega\partial_{\phi_p} \rightarrow \Omega_A\partial_{\varphi_A}$ in Eqs. (31) and (39); $F_\Omega^{(0)}\partial_{\phi_p} \rightarrow F_i^{(0)}\frac{\partial\Omega_A}{\partial p^i}\partial_{\varphi_A}$ in Eq. (34); and $\omega_m \rightarrow \omega_{m,k} = m\Omega_\phi + k\Omega_r$ in Eq. (43) [with k the integer labeling $h_{\alpha\beta}^{(n,m,k)}$, not to be confused with the height function $k(r^*)$]. We refer to Ref. [2] for more details.

III. LORENZ-GAUGE FIELD EQUATIONS

In the calculations in Refs. [7, 17, 18], and in much of this paper, we work in the Lorenz gauge. Here we review the Lorenz-gauge field equations as formulated in Ref. [9].

A. Four-dimensional form

We impose the Lorenz gauge condition

$$Z_\mu[\bar{\mathbf{h}}] = 0, \quad (46)$$

where $\mathbf{h}_{\mu\nu} := \mathbf{g}_{\mu\nu} - g_{\mu\nu}$ is the total perturbation and $\bar{\mathbf{h}}_{\mu\nu}$ is its trace reverse with respect to $g_{\mu\nu}$. This reduces the linearized Einstein tensor to

$$G_{\mu\nu}^{(1)}[\mathbf{h}] = -\frac{1}{2}E_{\mu\nu}[\bar{\mathbf{h}}]. \quad (47)$$

Following Ref. [47], in order to partially decouple the field equations, we use a modified operator

$$\check{E}_{\mu\nu} := E_{\mu\nu} - \frac{4M}{r^2} t_{(\mu} \check{Z}_{\nu)}, \quad (48)$$

where $t_\alpha := \partial_\alpha t$ and $\check{Z}_\alpha = (Z_r, 2Z_r, Z_\theta, Z_\phi)$ in Schwarzschild coordinates (t, r, θ, ϕ) ; note $\check{Z}_\alpha[\bar{h}]$ vanishes if the gauge condition is satisfied. The complete Einstein equation is then

$$\check{E}_{\mu\nu}[\bar{h}] = -16\pi T_{\mu\nu} + 2\check{G}_{\mu\nu}^{(2)}[\bar{h}, \bar{h}] + \mathcal{O}(|\bar{h}|^3). \quad (49)$$

Here $\check{G}_{\mu\nu}^{(2)}$ is given by $G_{\mu\nu}^{(2)}$ with Z_α set to zero.

Performing a multiscale expansion leads to a slightly modified version of the hierarchy (26) and (27),

$$\check{E}_{\mu\nu}^{(0)}[\bar{h}^{(1)}] = -16\pi T_{\mu\nu}^{(1)}, \quad (50)$$

$$\begin{aligned} \check{E}_{\mu\nu}^{(0)}[\bar{h}^{(2)}] &= -16\pi T_{\mu\nu}^{(2)} + 2\check{G}_{\mu\nu}^{(2,0)}[h^{(1)}, h^{(1)}] \\ &\quad - \check{E}_{\mu\nu}^{(1)}[\bar{h}^{(1)}]. \end{aligned} \quad (51)$$

The labels here have the same meaning as in the previous section: “(0)” on an operator indicates the operator with the replacement $\nabla_\alpha \rightarrow \nabla_\alpha^{(0)}$, and “(1)” indicates the term linear in \mathcal{V}_I . Explicitly, in terms of the operators in Eqs. (34) and (35),

$$\check{E}_{\mu\nu}^{(0)}[\bar{h}] = E_{\mu\nu}^{(1)}[\bar{h}] - \frac{4M}{r^2} t_{(\mu} \check{Z}_{\nu)}^{(1)}[\bar{h}] \quad (52)$$

with $\check{Z}_\alpha^{(1)} = (Z_r^{(1)}, 2Z_r^{(1)}, Z_\theta^{(1)}, Z_\phi^{(1)})$ in Schwarzschild coordinates.

Similarly, after the multiscale expansion, the gauge condition (46) becomes

$$Z_\mu^{(0)}[\bar{h}^{(1)}] = 0, \quad (53)$$

$$Z_\mu^{(0)}[\bar{h}^{(2)}] = -Z_\mu^{(1)}[\bar{h}^{(1)}]. \quad (54)$$

B. Tensor-harmonic decomposition

We next decompose the fields into tensor spherical harmonic modes, using the Barack-Lousto-Sago (BLS) basis of harmonics [47, 48]:

$$\bar{h}_{\alpha\beta}^{(n)} = \sum_{ilm} \frac{a_{i\ell}}{r} \bar{h}_{ilm}^{(n)}(r, \mathcal{J}_I) Y_{\alpha\beta}^{ilm}(r, \theta, \phi) e^{-im\phi_p}, \quad (55)$$

where $i = 1, \dots, 10$, $\ell \geq 0$, $m = -\ell, \dots, \ell$. The harmonics $Y_{\alpha\beta}^{ilm}$ provide an orthogonal basis for symmetric rank-2 tensors. They are given explicitly in Appendix B of Ref. [9]. $a_{i\ell}$ is a convenient numerical factor given by

$$a_{i\ell} = \begin{cases} \frac{1}{\sqrt{2}} & \text{for } i = 1, 2, 3, 6, \\ \frac{1}{\sqrt{2\ell(\ell+1)}} & \text{for } i = 4, 5, 8, 9, \\ \frac{1}{\sqrt{2(\ell-1)\ell(\ell+1)(\ell+2)}} & \text{for } i = 7, 10. \end{cases} \quad (56)$$

Following BLS, we have also pulled out a factor of $1/r$ in Eq. (55) to simplify the field equations.

We similarly decompose the source terms in Eqs. (50) and (51). Denoting the n th-order source term as $S_{\mu\nu}^{(n)}$, we write

$$S_{\mu\nu}^{(n)} = \sum_{ilm} S_{ilm}^{(n)}(r, \mathcal{J}_I) Y_{\mu\nu}^{ilm} e^{-im\phi_p}. \quad (57)$$

The mode number m appearing in the Fourier decomposition (41) is the same as the azimuthal mode number in the spherical harmonics, such that each mode in Eqs. (55) and (57) has a simple dependence on $(\phi - \phi_p)$:

$$Y_{\alpha\beta}^{ilm}(r, \theta, \phi) e^{-im\phi_p} = Y_{\alpha\beta}^{ilm}(r, \theta, 0) e^{im(\phi - \phi_p)}. \quad (58)$$

This implies that when a mode of $\bar{h}_{\alpha\beta}^{(n)}$ is evaluated on the worldline (where $r = r_p$, $\phi = \phi_p$, and $\theta = \pi/2$), it reduces to a function of \mathcal{J}_I , with no dependence on ϕ_p . The same is true of derivatives of $\bar{h}_{\alpha\beta}^{(n)}$, such as those that enter the self-force.

With these harmonic expansions, Eqs. (50) and (51) each separate into a set of ten ODEs for the coefficients $\bar{h}_{ilm}^{(n)}$, which read [48]

$$E_{ij\ell m}^{(0)} \bar{h}_{j\ell m}^{(n)} = -\frac{r f}{4a_{i\ell}} S_{ilm}^{(n)}. \quad (59)$$

Here the mode label j is summed over. The decomposed wave operator is given by

$$E_{ij\ell m}^{(0)} \bar{h}_{j\ell m} := \square_{\ell m}^{(0)} \bar{h}_{ilm} + \mathcal{M}_{ij}^{(0)} \bar{h}_{j\ell m}, \quad (60)$$

where

$$\begin{aligned} \square_{\ell m}^{(0)} := & -\frac{1}{4} \left[\partial_{r^*}^2 + i\omega_m (2H\partial_{r^*} + H') \right. \\ & \left. + (1 - H^2) \omega_m^2 - 4V_\ell(r) \right]. \end{aligned} \quad (61)$$

Here $H' := \frac{dH}{dr^*}$, and

$$V_\ell(r) = \frac{f}{4} \left(\frac{2M}{r^3} + \frac{\ell(\ell+1)}{r^2} \right). \quad (62)$$

$\mathcal{M}_{ij}^{(0)}$ with $i, j = 1, \dots, 10$ are a set of matrices composed of first-order differential operators that couple between the various $\bar{h}_{j\ell m}$'s. Note that the coupling is only between different j 's; there is no coupling between modes of different ℓ and m . Also note that the only effect of our added \check{Z}_ν term in Eq. (48) is to alter these coupling matrices (reducing the coupling). The explicit form of the coupling matrices can be found in Appendix A.

The source terms in the decomposed field equations (59) are

$$S_{ilm}^{(1)} = -16\pi T_{ilm}^{(1)}, \quad (63)$$

$$\begin{aligned} S_{ilm}^{(2)} &= -16\pi T_{ilm}^{(2)} + 2G_{ilm}^{(2,0)}[h^{(1)}, h^{(1)}] \\ &\quad - E_{ij\ell m}^{(1)} \bar{h}_{j\ell m}^{(1)}. \end{aligned} \quad (64)$$

The quadratic term, $G_{i\ell m}^{(2,0)}[h^{(1)}, h^{(1)}]$, is discussed in detail in Ref. [34]. Here we highlight the term involving $E_{ij\ell m}^{(1)}$, which is the decomposition of $\check{E}_{\mu\nu}^{(1)}$ in Eq. (51). This term represents the system's slow evolution acting as a source for the second-order metric perturbation. Explicitly,

$$E_{ij\ell m}^{(1)} \bar{h}_{j\ell m} := \square_{\ell m}^{(1)} \bar{h}_{i\ell m} + \mathcal{M}_{ij}^{(1)} \bar{h}_{j\ell m}, \quad (65)$$

where

$$\square_{\ell m}^{(1)} = \frac{1}{4} \left[(2H\partial_{r^*} + H') \bar{\partial}_\nu - (1 - H^2) (2i\omega_m \bar{\partial}_\nu + imF_\Omega^{(0)}) \right]. \quad (66)$$

The coupling matrices $\mathcal{M}_{ij}^{(1)}$ are given in Eq. (A17).

Similarly, at the level of modes, the gauge conditions (53) and (54) become

$$Z_{kj\ell}^{(0)} \bar{h}_{j\ell m}^{(1)} = 0 \quad (67)$$

and

$$Z_{kj\ell}^{(0)} \bar{h}_{j\ell m}^{(2)} = -Z_{kj\ell}^{(1)} \bar{h}_{j\ell m}^{(1)}, \quad (68)$$

where $k = 1, \dots, 4$. We give the operators $Z_{kj\ell}^{(n)}$ in Eqs. (A18) and (A19).

For $H = 0$ (i.e., t slicing), $E_{ij\ell m}^{(0)}$ and $Z_{kj\ell}^{(0)}$ are the same operators that appear in the standard frequency-domain Lorenz-gauge linearized field equations for a metric perturbation $\bar{h}_{\mu\nu} = \frac{a_{i\ell}}{r} \bar{h}_{i\ell m}(r) Y_{\mu\nu}^{i\ell m} e^{-i\omega t}$, as in Refs. [20, 49].

The equations in this section apply equally well for eccentric orbits, with the replacements $\omega_m \rightarrow \omega_{m,k} = m\Omega_\phi + k\Omega_r$ and $imF_\Omega^{(0)} \rightarrow -F_i^{(0)} \frac{\partial \omega_{m,k}}{\partial p_i}$.

C. Matrix form

For each ℓm mode, the field equations (59) represent 10 coupled ODEs. However, these ODEs partially decouple into a hierarchical structure; see Table I of Ref. [9]. Even-parity modes ($i = 1, \dots, 7$) decouple from odd-parity modes ($i = 8, 9, 10$). Moreover, the $i = 1, 3, 5, 6, 7$ modes decouple from the $i = 2, 4$ modes, and the $i = 9, 10$ modes decouple from the $i = 8$ mode; this allows one to calculate the $i = 2, 4$ modes from the $i = 1, 3, 5, 6, 7$ modes and the $i = 8$ mode from the $i = 9, 10$ modes. One can also often use the gauge condition to algebraically obtain some modes from others. The number of relevant modes is further reduced by the facts that (i) even-parity (odd-parity) modes vanish for $\ell + m$ odd ($\ell + m$ even), and (ii) $m < 0$ modes can be computed from $m > 0$ modes using $\bar{h}_{i\ell m} = (-1)^m (\bar{h}_{i\ell, -m})^*$.

It will be convenient to write these sets of equations in a canonical matrix form,

$$\mathcal{D}\psi := \frac{d^2\psi}{dr^2} + B \frac{d\psi}{dr} + A\psi = J, \quad (69)$$

where $\psi(r)$ and $J(r)$ are column vectors with d elements, and A and B are r -dependent $d \times d$ matrices. We further write this in first-order form as

$$\hat{\mathcal{D}}\hat{\psi} := \frac{d\hat{\psi}}{dr} + \hat{A}\hat{\psi} = \hat{J}, \quad (70)$$

where $\hat{\psi} = \begin{pmatrix} \psi \\ \partial_r \psi \end{pmatrix}$, $\hat{J}(r) = \begin{pmatrix} \mathbf{0}_d \\ J(r) \end{pmatrix}$ are $2d$ -vectors and

$$\hat{A} = \begin{pmatrix} \mathbf{0}_{d \times d} & -\mathbf{1}_{d \times d} \\ A & B \end{pmatrix}. \quad (71)$$

For our Lorenz-gauge field equations, the column vector $\psi_{\ell m}$ is

$$\psi = \begin{cases} (\bar{h}_9 \bar{h}_{10})^T & \ell \geq 2, \ell + m \text{ odd}, \\ (\bar{h}_1 \bar{h}_3 \bar{h}_5 \bar{h}_6 \bar{h}_7)^T & \ell \geq 2, \ell + m \text{ even}, m > 0, \\ (\bar{h}_1 \bar{h}_3 \bar{h}_5)^T & \ell \geq 2 \text{ even}, m = 0, \\ (\bar{h}_1 \bar{h}_3 \bar{h}_5 \bar{h}_6)^T & \ell = 1, m = 1, \\ \bar{h}_9 & \ell = 1, m = 0, \\ (\bar{h}_1 \bar{h}_3)^T & \ell = 0, \end{cases} \quad (72)$$

where T denotes the transpose and ℓm labels are suppressed. We then define the $2d$ -vector $\hat{\psi}_{\ell m} = (\psi_{\ell m}, \partial_r \psi_{\ell m})^T$. The matrices appearing in Eq. (71) are

$$A = \frac{1}{f^2} [\omega_m^2 (1 - H^2) + i\omega_m H' - 4V_\ell] \mathbf{1}_{d \times d} + \mathcal{M}_h, \quad (73a)$$

$$B = \frac{1}{f} \left(\frac{2M}{r^2} + 2i\omega_m H \right) \mathbf{1}_{d \times d} + \mathcal{M}_{\partial h}, \quad (73b)$$

where \mathcal{M}_h and $\mathcal{M}_{\partial h}$ are $d \times d$ matrices given in Appendix A.

We translate the sources in the same way. If $\bar{h}_{i\ell m}$ satisfies an equation $E_{ij\ell m}^{(0)} \bar{h}_{j\ell m} = -\frac{rf}{4a_{i\ell}} S_{i\ell m}$, as in Eq. (59), then the sources J in Eqs. (69) and (70) are

$$J = \frac{r}{a_{i\ell} f} \begin{cases} (S_9 S_{10})^T & \ell \geq 2, \ell + m \text{ odd}, m > 0, \\ (S_1 S_3 S_5 S_6 S_7)^T & \ell \geq 2, \ell + m \text{ even}, m > 0, \\ (S_1 S_3 S_5)^T & \ell \geq 2 \text{ even}, m = 0, \\ (S_1 S_3 S_5 S_6)^T & \ell = 1, m = 1, \\ S_9 & \ell = 1, m = 0, \\ (S_1 S_3)^T & \ell = 0, \end{cases} \quad (74)$$

again with ℓm labels suppressed.

For each ℓm , the modes that are missing from Eq. (72) can be obtained from the listed modes using the gauge condition (67) or (68). These ‘‘gauge modes’’ are \bar{h}_8 (for $\ell + m$ odd), \bar{h}_2 and \bar{h}_4 (for $\ell > 0$ and $\ell + m$ even), and \bar{h}_2 and \bar{h}_6 (for $\ell = 0$).

In the case of the second-order field, it will be useful to further divide the field into two pieces,

$$\hat{\psi}^{(2)} = \hat{\psi}^{(2,0)} + \hat{\psi}^{(1,1)}, \quad (75)$$

each satisfying its own field equation,

$$\hat{\mathcal{D}}\hat{\psi}^{(2,0)} = \hat{\mathcal{J}}^{(2,0)}, \quad (76)$$

$$\hat{\mathcal{D}}\hat{\psi}^{(1,1)} = \hat{\mathcal{J}}^{(1,1)}. \quad (77)$$

Here $\hat{\mathcal{J}}^{(2,0)}$ is constructed from the subset of source terms in Eq. (64) that do not involve the forcing functions $F_I^{(0)}$,

$$S_{ilm}^{(2,0)} = -16\pi T_{ilm}^{(2,0)} + 2G_{ilm}^{(2,0)}[h^{(1)}, h^{(1)}], \quad (78)$$

and $\hat{\mathcal{J}}^{(1,1)}$ is constructed from the subset of source terms that are linear in the forcing functions,

$$S_{ilm}^{(1,1)} = -16\pi T_{ilm}^{(1,1)} - E_{ijlm}^{(1)} \bar{h}_{jlm}^{(1)}. \quad (79)$$

In these expressions we have analogously split the stress-energy tensor into a piece ($T_{ilm}^{(2,0)}$) that is independent of $F_I^{(0)}$ and a piece ($T_{ilm}^{(1,1)}$) that is linear in it. In the present paper we will not require the explicit expressions for these two pieces; we only introduce the split to help organize discussions in later sections.

Despite the convenient split into $\hat{\psi}^{(2,0)}$ and $\hat{\psi}^{(1,1)}$, we stress that these fields are not actually independent: they are coupled through the gauge condition (68), which is only satisfied by the sum of the two fields.

D. Boundary conditions, punctures, and slicing transformations

Self-force calculations can encounter problematic divergent behavior in three regions: at the particle, near \mathcal{H}^+ , and near \mathcal{I}^+ .⁶ The nature of the problem depends on the particular formulation of the small- ε expansion, on the choice of gauge, and on the choice of time foliation. Punctures provide a practical way of enforcing physical boundary conditions in the presence of these divergences.

To motivate the use of punctures, we first recall their use in controlling the divergence at the particle, which is the most familiar problem. Fundamentally, an expansion in the limit $\varepsilon \rightarrow 0$ (at fixed external length scales) breaks down at distances $\sim \varepsilon$ from the small companion; there, the gravity of the small body dominates over the external gravity. Through a local analysis in that region, using the method of matched asymptotic expansions, one finds the correct local behavior of the physical solution [1]. The form of that solution, outside the body, is

$$h_{\mu\nu}^{(n)} = h_{\mu\nu}^{S(n)} + h_{\mu\nu}^{R(n)}. \quad (80)$$

The self-field $h_{\mu\nu}^{S(n)}$ captures local information about the body's multipole structure and diverges if analytically extended down to the body's representative worldline. The regular field $h_{\mu\nu}^{R(n)}$ is a vacuum solution that depends on global boundary conditions and is smooth when analytically extended to the worldline.

We then adopt an asymptotic matching condition, which is a type of boundary condition: near the representative worldline, the metric perturbations must recover the local form obtained from matched asymptotic expansions. The point-mass representation (6) and a puncture scheme are two differing ways to enforce this condition. Both methods use the analytical extension of Eq. (80) down to the worldline. The point-mass representation enforces the matching condition by defining source terms for $h_{\mu\nu}^{(n)}$ such that all solutions to the inhomogeneous field equation recover the correct local form (80); we refer to Ref. [37] for further discussion. A puncture scheme instead imposes the matching condition by directly using the local form (80). We construct a local approximation to $h_{\mu\nu}^{S(n)}$, called a puncture field $h_{\mu\nu}^{P(n)}$, and then solve field equations for the residual field $h_{\mu\nu}^{R(n)} := h_{\mu\nu}^{(n)} - h_{\mu\nu}^{P(n)}$. In our generic matrix form, we write these field equations as

$$\hat{\mathcal{D}}\hat{\psi}^R = \hat{\mathcal{J}} - \hat{\mathcal{D}}\hat{\psi}^P =: \hat{\mathcal{J}}^{\text{eff}}. \quad (81)$$

The puncture field is made to vanish outside some region around the particle, such that $\hat{\psi}^R$ becomes the physical field outside that region. By solving Eq. (81) with physical boundary conditions at \mathcal{H}^+ and \mathcal{I}^+ and adding the puncture, we then obtain a total field $\hat{\psi}^R + \hat{\psi}^P$ that necessarily satisfies the matching condition. We note that the punctures $h_{\mu\nu}^{P(n)}$ and residual fields $h_{\mu\nu}^{R(n)}$ possess the same multiscale form as $h_{\mu\nu}^{(n)}$ because $h_{\mu\nu}^{P(n)}$ is an explicit function of the orbital trajectory.

This illustrates how a puncture scheme is simply a method of imposing a boundary condition. Suppose, more generally, we are given the boundary condition that the total physical solution to Eq. (69) must take the form $\hat{\psi}^R + \hat{\psi}^S$ near some boundary, where $\hat{\psi}^S$ is a specific particular solution (possibly singular at the boundary) and $\hat{\psi}^R$ is a homogeneous solution that is regular at the boundary. If we construct a puncture $\hat{\psi}^P$ that approximates $\hat{\psi}^S$ sufficiently well, and if we impose regular boundary conditions on the residual $\hat{\psi}^R$, then solving Eq. (81) and adding $\hat{\psi}^P$ yields a solution to Eq. (69) that satisfies the given boundary conditions. We apply this method at both outer boundaries, \mathcal{H}^+ and \mathcal{I}^+ .

Sections V.F–H in Ref. [9] discuss the behavior of the second-order physical solution near \mathcal{H}^+ and \mathcal{I}^+ . Here we briefly review and add some details to that discussion. We follow Ref. [9] in using a label “[s]” to indicate the slicing in which a mode is defined.

To frame the discussion, we first note how homogeneous solutions depend on slicing. For a homogeneous solution, the mode coefficients in generic s slicing are re-

⁶ Additionally, regular perturbation theory diverges on long time scales [33]. This failure is overcome using a multiscale expansion, as we use here, or using a self-consistent expansion [46] (if the latter is extended to account for the black hole's slow evolution, as described in Ref. [9]).

lated to those in t slicing by

$$\psi_{[s]} = \psi_{[t]} e^{-i\omega k(r^*)}, \quad (82)$$

implying

$$\partial_r \psi_{[s]} = (\partial_r \psi_{[t]} - i\omega f^{-1} H \psi_{[t]}) e^{-i\omega k(r^*)}. \quad (83)$$

(We omit the subscript m on ω for succinctness and because the discussion in this section applies equally well for eccentric orbits.) In matrix form,

$$\hat{\psi}_{[s]} = \begin{pmatrix} \mathbf{1}_{d \times d} & \mathbf{0}_{d \times d} \\ -i\omega f^{-1} H \mathbf{1}_{d \times d} & \mathbf{1}_{d \times d} \end{pmatrix} \hat{\psi}_{[t]} e^{-i\omega k(r^*)}, \quad (84)$$

where d is the dimension of the vector ψ .

Homogeneous solutions regular at \mathcal{H}^+ behave like

$$\hat{\psi}_{[v]} \sim f^0 \quad (85)$$

for $r \rightarrow 2M$ in v slicing. Equation (84) therefore implies that such solutions behave as

$$\hat{\psi}_{[t]} \sim \begin{pmatrix} f^0 \\ i\omega f^{-1} \end{pmatrix} e^{-i\omega r^*} \quad (86)$$

in t slicing, where it is understood that the two entries in the vector indicate the scaling of the top and bottom d rows in $\hat{\psi}_{[t]}$, respectively. Homogeneous solutions regular at \mathcal{S}^+ behave like

$$\hat{\psi}_{[u]} \sim r^0 \quad (87)$$

at large r [corresponding to $h_{\mu\nu} \sim 1/r$ because of the rescaling by r in Eq. (55)]. Equation (84) therefore implies

$$\hat{\psi}_{[t]} \sim e^{+i\omega r^*} \quad (88)$$

in t slicing.

At first order, outside the source region, the physical, retarded solutions are homogeneous. They therefore must satisfy the regularity conditions at \mathcal{H}^+ and \mathcal{S}^+ as described in the preceding paragraph.

At second order, the boundary conditions are more complicated because of the behavior of the source terms. Away from the particle, the quadratic source term $G_{\mu\nu}^{(2,0)}$ is made up of products of homogeneous solutions. At large r , in generic s slicing,

$$G_{\mu\nu}^{(2,0)} \sim \frac{e^{i\omega[r^* - k(r^*)]}}{r^2}, \quad (89)$$

implying a source $\hat{J}^{(2,0)} \sim \frac{e^{i\omega[r^* - k(r^*)]}}{r}$ in the equation (76). In u slicing (for which $k = r^*$), the oscillations are eliminated, but the falloff is unaffected. All solutions are then singular at \mathcal{S}^+ , behaving as

$$\psi_{[u]}^{(2,0)} \sim \ln r \quad (90)$$

for $\omega \neq 0$ modes or as

$$\psi_{[u]}^{(2,0)} \sim r \ln r \quad (91)$$

for certain $\omega = 0$ modes. This behaviour was discussed in detail in Ref. [33] and will be returned to in a later paper.

At the opposite boundary, near the horizon,

$$G_{\mu\nu}^{(2,0)} \sim e^{-i\omega[r^* + k(r^*)]}, \quad (92)$$

meaning $\hat{J}^{(2,0)} \sim f^{-1}$ at the horizon in v slicing (for which $k = -r^*$). The physical solution in the Lorenz gauge then turns out to be singular at the horizon despite the smoothness of the physical source $G_{\mu\nu}^{(2,0)}$. Again, this will be discussed in a future paper.

Next, we consider the source $G_{\mu\nu}^{(1,1)}[h^{(1)}]$ given in Eq. (33) and corresponding source $\hat{J}^{(1,1)}$ in Eq. (77). If we choose t slicing, then $H = 0$, implying

$$\hat{J}_{[t]}^{(1,1)} \sim \omega F_{\Omega}^{(0)} r^* e^{i\omega r^*} \quad (93)$$

at large r , and so the field sourced by $\hat{J}_{[t]}^{(1,1)}$ behaves as $\hat{\psi}_{[t]}^{(1,1)} \sim r^2 e^{i\omega r^*}$. On the other hand, if we choose u slicing, then $H = 1$, implying

$$\hat{J}_{[u]}^{(1,1)} \sim 1/r^2 \quad (94)$$

at large r , and so $\hat{\psi}_{[u]} \sim r^0$. Similarly, the source $\hat{J}_{[t]}^{(1,1)}$ is ill behaved at the horizon, scaling as

$$\hat{J}_{[t]}^{(1,1)} \sim r^* f^{-1} e^{-i\omega r^*}, \quad (95)$$

while the source $\hat{J}_{[v]}^{(1,1)}$ is smooth at the horizon, behaving as

$$\hat{J}_{[v]}^{(1,1)} \sim f^0. \quad (96)$$

Fields sourced by $\hat{J}_{[t]}^{(1,1)}$ and fields sourced by $\hat{J}_{[v]}^{(1,1)}$ therefore have very different behavior near the horizon. We discuss that behavior in Sec. VIII.

In cases where the physical solution is singular at a boundary, we introduce a puncture at that boundary as described above. Even in cases where a puncture is not strictly required, we can introduce one to increase the falloff rate of the effective source \hat{J}^{eff} toward the boundaries; this is beneficial because it improves the efficiency of integration over the source. In later sections we discuss the requirements on the puncture.

IV. TEUKOLSKY EQUATIONS

In the Teukolsky formalism, instead of directly dealing with metric perturbations, one considers perturbations of

a Weyl curvature scalar. We shall focus on the curvature scalar ψ_4 , defined as

$$\psi_4 = C_{\alpha\beta\gamma\delta} n^\alpha \bar{m}^\beta n^\gamma \bar{m}^\delta. \quad (97)$$

Here, the overbar denotes complex conjugation, $C_{\alpha\beta\gamma\delta}$ is the Weyl curvature tensor, and the vectors are elements of a Newman-Penrose null tetrad $\{l^\alpha, n^\alpha, m^\alpha, \bar{m}^\alpha\}$ [50, 51].

We will specifically focus on *linear* perturbations of the Weyl scalar, meaning that for a given metric perturbation $h_{\alpha\beta}$, we consider ψ_4 to be (with an abuse of notation) the piece of the Weyl curvature that is linear in $h_{\alpha\beta}$:

$$\psi_4[h] = C_{\alpha\beta\gamma\delta}^{(1,0)}[h] n^\alpha \bar{m}^\beta n^\gamma \bar{m}^\delta. \quad (98)$$

Here the tetrad legs are defined in the background spacetime, and the linearized Weyl tensor $C_{\alpha\beta\gamma\delta}^{(1,0)}$ is defined in analogy with the linearized Einstein tensor $G_{\alpha\beta}^{(1,0)}[h]$ of previous sections. Our ψ_4 corresponds to the quantity $\delta\psi_4$ in Ref. [34], but with the covariant derivative ∇ replaced with its zeroth-order version $\nabla^{(0)}$ from Eq. (31). Analogously, we define the linearized curvature scalar $\psi_0[h] = C_{\alpha\beta\gamma\delta}^{(1,0)}[h] l^\alpha m^\beta l^\gamma m^\delta$.

We note that our formulation in this section remains specialised to Schwarzschild spacetime (though the extension to Kerr, starting from Ref. [35], is immediate).

A. “Reduced” Teukolsky equations

Given an equation $G_{\mu\nu}^{(1,0)}[h] = S_{\mu\nu}$ for a metric perturbation $h_{\mu\nu}$, we can obtain an associated spin-weight $s = \pm 2$ Teukolsky master equation [52],

$${}_s\mathcal{O} {}_s\psi = {}_sS, \quad (99)$$

where ${}_s\mathcal{O}$ is the spin-weight s Teukolsky (wave) operator, ${}_s\psi$ is constructed from $h_{\mu\nu}$, and ${}_sS$ is constructed from $S_{\mu\nu}$.

The specific relationships between variables depends on the choice of tetrad. We work with the Kinnersley tetrad [53], in which ${}_{-2}\psi = \rho^{-4}\psi_4$ and ${}_{-2}\mathcal{O} = 2r^2\rho^{-4}\mathcal{O}\rho^4$, where \mathcal{O} is the second-order differential operator

$$\begin{aligned} \mathcal{O} := & [\mathbb{P}' - (2s+1)\rho'] (\mathbb{P} - \rho) - \delta'\delta \\ & - \frac{1}{2} [(6s+2) + 4s^2] \psi_2, \end{aligned} \quad (100)$$

with $\rho = -1/r$, $\rho' = f/(2r)$, and $\psi_2 = -M/r^3$. Similarly, the source for ${}_{-2}\psi$ is given by ${}_{-2}T = 2r^2\rho^{-4}\mathcal{S}[S_{\alpha\beta}]$,

where⁷

$$\begin{aligned} \mathcal{S}[S_{\alpha\beta}] = & \frac{1}{2} \delta' [(\mathbb{P}' - 2\bar{\rho}') S_{(n\bar{m})} - \delta' S_{nn}] \\ & + \frac{1}{2} (\mathbb{P}' - 4\rho' - \bar{\rho}') [\delta' S_{(n\bar{m})} - (\mathbb{P}' - \bar{\rho}') S_{\bar{m}\bar{m}}]. \end{aligned} \quad (101)$$

In these definitions, we adopt Geroch-Held-Penrose (GHP) notation, following the conventions of [2] (simplified with $\tau = \tau' = 0$ in a Schwarzschild background). The GHP derivatives \mathbb{P} , \mathbb{P}' , δ , and δ' , along with a brief review of the GHP formalism, can be found in Appendix C 2.

The mode decomposition likewise depends on the choice of null tetrad. Again working with the Kinnersley tetrad, we write our separation ansatz as

$$\begin{aligned} {}_s\psi = & r^{-(2s+1)} f^{-s} \\ & \times \sum_{\ell=2}^{\infty} \sum_{m=-\ell}^{\ell} {}_sR_{\ell m}(r, \mathcal{I}_I) {}_sY_{\ell m}(\theta, \phi) e^{-im\phi_p}, \end{aligned} \quad (102)$$

where ${}_sY_{\ell m}(\theta, \phi)$ are spin-weighted spherical harmonics [54]; these are straightforwardly related to the tensor harmonics $Y_{\mu\nu}^{i\ell m}$ that we use for the Lorenz-gauge metric perturbations [34]. The radial Teukolsky function, ${}_sR_{\ell m}(r)$, satisfies the ordinary differential equation

$$\begin{aligned} & \left(r^2 f \frac{d^2}{dr^2} + 2 [M - s(r-M) + i\omega r^2 H] \frac{d}{dr} \right. \\ & \left. + \frac{r^2}{f} [\omega^2 (1-H^2) + i\omega H' - {}_sV_{\ell m}(r)] \right) {}_sR_{\ell m}(r) \\ & = {}_sS_{\ell m}(r). \end{aligned} \quad (103)$$

Here, $\omega = m\Omega$, the Teukolsky potential reads

$$\begin{aligned} {}_sV_{\ell m}(r) := & \frac{2is\omega}{r^2} [fr(1-H) - M(1+H)] \\ & + \frac{f}{r^2} \left[\ell(\ell+1) - s(s+1) + \frac{2M(s+1)}{r} \right], \end{aligned} \quad (104)$$

and the source mode coefficients are defined from

$${}_sS = - \sum_{\ell=2}^{\infty} \sum_{m=-\ell}^{\ell} {}_sS_{\ell m}(r, \mathcal{I}_I) {}_sY_{\ell m}(\theta, \phi) e^{-im\phi_p}. \quad (105)$$

The explicit form of the source for the case we shall explore in this work can be found in Appendix C.

The factor $r^{-(2s+1)} f^{-s}$ in the mode ansatz (102) is introduced for the purposes of numerical integration of the radial Teukolsky equation. This was first introduced in the context of hyperboloidal slicing for the Teukolsky

⁷ In [2], this is denoted S_4 .

equation in [31], and has been further utilised in the subsequent works [55–57]. Without this rescaling, the potential would only fall off as $1/r$ toward infinity and would not vanish at the horizon. Therefore, the potential would be long-ranged, akin to the Coulomb potential. For any non-zero spin-weight, one could not accurately compute solutions of the homogeneous Teukolsky equation due to numerical round-off error either near the horizon or towards infinity. Hence, in rescaling the master function in accordance with its asymptotic behaviour, we obtain a short-ranged potential in Eq. (104) that now falls off as f near the horizon and r^{-2} near null infinity. Furthermore, our use of hyperboloidal slicing eliminates the oscillatory behaviour of the radial function toward infinity and the horizon, which increases the efficiency of the numerical solver.

As we did for the Lorenz-gauge field equations, we express our radial Teukolsky equation in the form of Eq. (69). The column vector ψ in Eq. (69) reduces to 1 element with $\psi(r) = {}_s R_{\ell m}(r)$, with A and B given by

$$A = \frac{\omega^2(1-H^2) - {}_s V_{\ell m}(r)}{f^2},$$

$$B = \frac{1}{f} \left(\frac{2M}{r^2} + 2i\omega H + \frac{2s(r-M)}{r^2} \right). \quad (106)$$

Similarly, the source reduces to $J(r) = r^{2s-1} f^{s-1} {}_s S_{\ell m}(r, \mathcal{I}_I)$.

All of the above formulas apply for each field

$${}_{-2}\psi^{(n)} = \rho^{-4} \psi_4[h^{(n)}]. \quad (107)$$

In analogy with Eq. (75), we split the second-order field into two pieces,

$${}_{-2}\psi^{(2,0)} = \rho^{-4} \psi_4[h^{(2,0)}], \quad (108)$$

$${}_{-2}\psi^{(1,1)} = \rho^{-4} \psi_4[h^{(1,1)}]. \quad (109)$$

Again, all the formulas in this section apply to each of these pieces. In analogy with Eqs. (76) and (77), the radial coefficients in the mode decompositions of ${}_{-2}\psi^{(2,0)}$ and ${}_{-2}\psi^{(1,1)}$ satisfy radial Teukolsky equations with sources constructed from

$$S_{\mu\nu}^{(2,0)} = 8\pi T_{\mu\nu}^{(2,0)} - G_{\mu\nu}^{(2,0)}[h^{(1)}, h^{(1)}], \quad (110)$$

$$S_{\mu\nu}^{(1,1)} = 8\pi T_{\mu\nu}^{(1,1)} - G_{\mu\nu}^{(1,1)}[h^{(1)}]. \quad (111)$$

Note that our field ${}_{-2}\psi^{(2)}$ does not represent the second-order term in an expansion of the spacetime's full Weyl scalar. Such an expansion would include quadratic terms constructed from $h_{\mu\nu}^{(1)}$ and from perturbations of the tetrad legs, while our field involves only the piece that is linear in $h_{\mu\nu}^{(1)}$. We refer to Ref. [35] for a thorough discussion; there, we refer to the field equation for our linear ${}_{-2}\psi^{(2)}$ as the *reduced* second-order Teukolsky equation. Similar comments apply to ${}_{-2}\psi^{(1,1)}$.

B. Boundary conditions

The core aspects of Sec. III D carry over to the Teukolsky case, including the use of punctures. However, solutions of the radial Teukolsky equation do behave in significantly different ways near the boundaries than Lorenz-gauge metric perturbations. Here we do not attempt a comprehensive summary of the behavior of sourced solutions, comparable to Sec. III D. Instead, we only highlight the behavior of a basis of homogeneous solutions, analogous to Eqs. (85)–(88). This basis is made up of a pair of solutions that are respectively purely ingoing at \mathcal{H}^+ and purely outgoing at \mathcal{I}^+ . In the usual Teukolsky nomenclature these are referred to as ‘in’ and ‘up’ solutions [2].

The ‘in’ solution is regular at the horizon and has the near-boundary behavior

$$\hat{\psi}_{[t]}^- \sim \begin{cases} e^{-i\omega r^*}, & r \rightarrow 2M, \\ e^{i\omega r^*} + r^{2s} e^{-i\omega r^*}, & r \rightarrow \infty. \end{cases} \quad (112)$$

Conversely, the ‘up’ solution is regular at \mathcal{I}^+ and behaves as

$$\hat{\psi}_{[t]}^+ \sim \begin{cases} e^{-i\omega r^*} + f^s e^{i\omega r^*}, & r \rightarrow 2M, \\ e^{i\omega r^*}, & r \rightarrow \infty. \end{cases} \quad (113)$$

These limiting behaviors can be verified by applying the rescaling in Eq. (102) to the form of the master functions in Table 1 of Ref. [58].

At the boundaries where these homogeneous solutions represent physical waves created by a compact source, they have the same behavior as the Lorenz-gauge metric perturbations. However, they differ in important ways at the opposite boundaries. For the spin weight we focus on ($s = -2$), Eq. (112) shows that in the ‘in’ solution, the incoming portion of the solution at large r decays rapidly, as r^{-4} ; and Eq. (113) shows that in the ‘up’ solution, the outgoing portion of the solution at the horizon blows up there. Homogeneous Lorenz-gauge perturbations, on the other hand, behave like $s = 0$ solutions in Eqs. (112) and (113): a solution that is a pure ingoing wave at the horizon is a mix of ingoing ($r^0 e^{-i\omega r^*}$) and outgoing ($r^0 e^{+i\omega r^*}$) waves at infinity; and a solution that is a pure outgoing wave at infinity is a mix of ingoing and (bounded) outgoing waves at the horizon. The more intricate behaviour of the homogeneous Teukolsky solutions has important knock-on effects for inhomogeneous solutions with non-compact sources, explained in Sec. VIII D.

V. PUNCTURE SCHEME WITH SMOOTH SLICING AND WINDOWED PUNCTURES

Before considering our worldtube scheme with multiple distinct regions, we first consider a simpler but less computationally convenient method. We assume the time function s is smooth, and if there are punctures, we

use window functions to make them transition to zero at some distance from the particle or from the boundary where they are used. This is an extension of the window-function method that one of us applied to first-order Lorenz-gauge calculations in Ref. [20], now allowing for alternative time functions and noncompact sources.

We keep our discussion generic in this section, making it equally valid for eccentric orbits as for quasicircular orbits.

A. Generic source

We consider a generic set of coupled first-order radial ODEs written in the matrix form (70), reproduced here for convenience:

$$\hat{\mathcal{D}}\hat{\psi} := \frac{d\hat{\psi}}{dr} + \hat{A}\hat{\psi} = \hat{J}, \quad (114)$$

where $\hat{\psi} = (\psi, \partial_r \psi)^T$ and $\hat{J} = (\mathbf{0}_d, J)^T$ are column vectors of length $2d$. These can be the Lorenz-gauge field equations, Teukolsky equations, or another set of equations. We let the domain of the solutions to (114) be $r \in (2M, \infty)$, and we assume that \hat{J} is integrable (or well defined as a distribution) in that domain and falls off sufficiently rapidly toward the boundaries (a condition that will be enforced below through the use of boundary punctures).

Now we seek a solution to Eq. (114) subject to physical boundary conditions at $r = 2M$ and $r = \infty$. We can construct the solution using the method of variation of parameters [59]. Take the homogeneous version of Eq. (114) ($\hat{J} = 0$), which has $2d$ independent solutions. We denote by $\hat{\psi}_{k-}$, with $k = 1, \dots, d$, the d independent homogeneous solutions that obey desired boundary conditions at $r = 2M$, and by $\hat{\psi}_{k+}$ the d independent solutions that obey desired boundary conditions at infinity. For concreteness, for $\omega \neq 0$ modes, $\hat{\psi}_{k-}$ will represent ingoing waves regular at the future horizon, and $\hat{\psi}_{k+}$ will represent outgoing waves at future null infinity. For $\omega = 0$ modes, $\hat{\psi}_{k-}$ will be homogeneous solutions regular at the horizon, and $\hat{\psi}_{k+}$ will be asymptotically flat homogeneous solutions. Using these solutions we define a $2d \times 2d$ matrix of homogeneous solutions,

$$\Phi := \left(\hat{\psi}_{1-}, \dots, \hat{\psi}_{d-}, \hat{\psi}_{1+}, \dots, \hat{\psi}_{d+} \right), \quad (115)$$

satisfying

$$\frac{d}{dr}\Phi + \hat{A}\Phi = 0. \quad (116)$$

Appendix B reviews the construction of the basis of homogeneous solutions.

In terms of Φ the general solution to Eq. (114) can be written as

$$\hat{\psi} = \Phi \left(\int_{2M}^r dr' \Phi^{-1}(r') \hat{J}(r') + a \right), \quad (117)$$

with a an arbitrary, constant $2d$ -vector. Writing Φ in the form

$$\Phi = (\Phi_-, \Phi_+) \quad (118)$$

with $\Phi_{\pm} = (\hat{\psi}_{1\pm}, \dots, \hat{\psi}_{d\pm})$ a $2d \times d$ matrix, we can also write Eq. (117) as

$$\begin{aligned} \hat{\psi} = & \Phi_- \left(\int_{2M}^r dr' \Phi_{\text{top}}^{-1} \hat{J} + a_{\text{top}} \right) \\ & + \Phi_+ \left(\int_{2M}^r dr' \Phi_{\text{bot}}^{-1} \hat{J} + a_{\text{bot}} \right). \end{aligned} \quad (119)$$

Here and below, ‘top’ and ‘bot’ refer to the top or bottom d rows of a matrix with $2d$ rows, and $\Phi_{\text{top/bot}}^{-1}$ specifically denotes the top or bottom d rows of the $2d \times 2d$ matrix Φ^{-1} .

B. Compact source

First consider the case in which the source has compact support. This is the typical situation at first order, in which the point-particle, frequency-domain source is confined to a single radius (for a circular orbit) or to the libration region (for an eccentric orbit [60]), and the effective, punctured source is confined to a region around the particle.

If the source is supported between some r_{\min} and r_{\max} , then outside of that region, the physical, retarded field must reduce to a linear combination of the appropriate homogeneous solutions:

$$\hat{\psi}^{\text{ret}} = \begin{cases} \Phi_+ c_+ & \text{for } r > r_{\max}, \\ \Phi_- c_- & \text{for } r < r_{\min}, \end{cases} \quad (120)$$

for some constant d -vectors c_{\pm} .

Explicitly evaluating the general solution (119) outside the source region, we find

$$\hat{\psi}(r < r_{\min}) = \Phi_- a_{\text{top}} + \Phi_+ a_{\text{bot}}, \quad (121)$$

$$\begin{aligned} \hat{\psi}(r > r_{\max}) = & \Phi_- \left(\int_{2M}^{\infty} dr' \Phi_{\text{top}}^{-1} \hat{J} + a_{\text{top}} \right) \\ & + \Phi_+ \left(\int_{2M}^{\infty} dr' \Phi_{\text{bot}}^{-1} \hat{J} + a_{\text{bot}} \right). \end{aligned} \quad (122)$$

The boundary conditions (120) hence imply

$$a = \left(- \int_{2M}^{\infty} dr' \Phi_{\text{top}}^{-1}(r') \hat{J}(r'), \mathbf{0}_d \right)^T. \quad (123)$$

Therefore the retarded solution is

$$\hat{\psi}^{\text{ret}} = \Phi \mathbf{v}, \quad (124)$$

where \mathbf{v} is the $2d$ -vector

$$\mathbf{v} = \left(- \int_r^{\infty} dr' \Phi_{\text{top}}^{-1} \hat{J}, \int_{2M}^r dr' \Phi_{\text{bot}}^{-1} \hat{J} \right)^T. \quad (125)$$

Note that $\mathbf{v} = (c_-, 0)^T$ for $r < r_{\min}$ and $\mathbf{v} = (0, c_+)^T$ for $r > r_{\max}$; or, restated as an equation for c_{\pm} ,

$$c_+ = \int_{2M}^{r_{\max}} dr' \Phi_{\text{bot}}^{-1} \hat{J}, \quad (126)$$

$$c_- = - \int_{r_{\min}}^{\infty} dr' \Phi_{\text{top}}^{-1} \hat{J}. \quad (127)$$

For a given source \hat{J} , we will refer to (124) as the retarded integral of \hat{J} . If \hat{J} has compact support, then this also represents the physical retarded solution; if \hat{J} has non-compact support, then the retarded integral of it may or may not represent the physical retarded solution.

C. Noncompact, punctured source

Now we consider the case where the source is noncompact, extending to the boundaries. This is the situation at second order.

As described in Sec. III D, the boundary conditions on the physical field are

$$\hat{\psi}^{\text{ret}} = \begin{cases} \hat{\psi}_+^{\text{S}} + \Phi_+ c_+ & \text{for } r \rightarrow \infty, \\ \hat{\psi}_-^{\text{S}} + \Phi_- c_- & \text{for } r \rightarrow 2M, \end{cases} \quad (128)$$

for some constant d -vectors c_{\pm} . $\hat{\psi}_{\pm}^{\text{S}}$ is a given particular solution to

$$\hat{D}\hat{\psi}_{\pm}^{\text{S}} = \hat{J}, \quad (129)$$

and it is typically singular at the boundary where it is used.

We can enforce the boundary conditions (128) using punctures. Let the punctures $\hat{\psi}_{\pm}^{\text{P}}$ approximate $\hat{\psi}_{\pm}^{\text{S}}$ near the boundaries and then transition smoothly to zero. Define $\hat{\psi}^{\text{P}} = \hat{\psi}_+^{\text{P}} + \hat{\psi}_-^{\text{P}}$ (plus a puncture at the particle if appropriate). The residual field $\hat{\psi}^{\text{R}} = \hat{\psi}^{\text{ret}} - \hat{\psi}^{\text{P}}$ then satisfies

$$\hat{D}\hat{\psi}^{\text{R}} = \hat{J} - \hat{D}\hat{\psi}^{\text{P}} =: \hat{J}^{\text{eff}}. \quad (130)$$

To enforce (128), we adopt the retarded solution to this equation, taking the retarded integral (124) of \hat{J}^{eff} :

$$\begin{aligned} \hat{\psi}^{\text{R}} = & -\Phi_- \int_r^{\infty} dr' \Phi_{\text{top}}^{-1} \hat{J}^{\text{eff}} \\ & + \Phi_+ \int_{2M}^r dr' \Phi_{\text{bot}}^{-1} \hat{J}^{\text{eff}}. \end{aligned} \quad (131)$$

If \hat{J}^{eff} falls off sufficiently quickly toward the boundaries, then this solution for $\hat{\psi}^{\text{R}}$ approximates the homogeneous solutions $\Phi_{\pm} c_{\pm}$ near the boundaries, fixing the values of the coefficients c_{\pm} and ensuring that the total field $\hat{\psi}^{\text{P}} + \hat{\psi}^{\text{R}}$ takes the form in (128).

To see that we are correct in using the retarded integral (131), start by assuming we know the particular

solutions $\hat{\psi}_{\pm}^{\text{S}}$ exactly. In that case we can adopt punctures $\hat{\psi}_{\pm}^{\text{Pexact}} = \hat{\psi}_{\pm}^{\text{S}} \mathcal{W}_{\pm}$, where \mathcal{W}_{\pm} is a window function that is identically equal to 1 in a neighborhood of the worldline and transitions to zero at some finite distance from the worldline. The effective source then has compact support, identically vanishing in a neighborhood of the boundaries. In this circumstance, we rename the $\hat{\psi}^{\text{R}}$ in Eq. (131) as $\hat{\psi}^{\text{Rexact}}$. Near $r = 2M$, where $\hat{J}^{\text{eff}} = 0$, $\hat{\psi}^{\text{Rexact}}$ becomes the homogeneous solution

$$\hat{\psi}^{\text{Rexact}} = -\Phi_- \int_{2M}^{\infty} dr' \Phi_{\text{top}}^{-1} \hat{J}^{\text{eff}}, \quad (132)$$

implying the unknown constant c_- in Eq. (128) is $c_- = - \int_{2M}^{\infty} dr' \Phi_{\text{top}}^{-1} \hat{J}^{\text{eff}}$. Analogously, near $r \rightarrow \infty$ we have

$$\hat{\psi}^{\text{Rexact}} = \Phi_+ \int_{2M}^{\infty} dr' \Phi_{\text{bot}}^{-1} \hat{J}^{\text{eff}}, \quad (133)$$

implying c_+ in Eq. (128) is $c_+ = \int_{2M}^{\infty} dr' \Phi_{\text{bot}}^{-1} \hat{J}^{\text{eff}}$.

Now consider the case we encounter in practice, in which we only know $\hat{\psi}_{\pm}^{\text{S}}$ approximately, up to some finite order in a series expansion around $r \rightarrow \infty$ or around $r = 2M$. Suppose we use such approximations as punctures $\hat{\psi}_{\pm}^{\text{P}}$, such that

$$\hat{\psi}_{\pm}^{\text{P}} = \hat{\psi}_{\pm}^{\text{Pexact}} + \Delta\hat{\psi}_{\pm}^{\text{P}} \quad (134)$$

for some $\Delta\hat{\psi}_{\pm}^{\text{P}}$. For the puncture scheme to be useful, the total field must be robust under this change in the punctures, at least so long as $\Delta\hat{\psi}_{\pm}^{\text{P}}$ is sufficiently small in the limit to the boundary; the change in the punctures must be exactly counterbalanced by a commensurate change in the residual field, leaving the total field unaltered.

Let us assess the restrictions this imposes on $\Delta\hat{\psi}_{\pm}^{\text{P}}$, and whether we can safely use the retarded integral (131) for $\hat{\psi}^{\text{R}}$. The new residual field, $\hat{\psi}^{\text{R}} = \hat{\psi}^{\text{ret}} - \hat{\psi}^{\text{P}}$, satisfies

$$\hat{D}\hat{\psi}^{\text{R}} = \hat{J} - \hat{D}\hat{\psi}^{\text{P}} = \hat{J} - \hat{D}\hat{\psi}^{\text{Pexact}} - \hat{D}\Delta\hat{\psi}^{\text{P}}. \quad (135)$$

Therefore the *change* in the residual field, $\Delta\hat{\psi}^{\text{R}} = \hat{\psi}^{\text{R}} - \hat{\psi}^{\text{Rexact}}$, satisfies

$$\hat{D}\Delta\hat{\psi}^{\text{R}} = -\hat{D}\Delta\hat{\psi}^{\text{P}}. \quad (136)$$

The retarded integral is

$$\begin{aligned} \Delta\hat{\psi}^{\text{R}} = & \Phi_- \int_r^{\infty} dr' \Phi_{\text{top}}^{-1} \hat{D}\Delta\hat{\psi}^{\text{P}} \\ & - \Phi_+ \int_{2M}^r dr' \Phi_{\text{bot}}^{-1} \hat{D}\Delta\hat{\psi}^{\text{P}}. \end{aligned} \quad (137)$$

Using $\hat{D}\Delta\hat{\psi}^{\text{P}} = \frac{d}{dr}\Delta\hat{\psi}^{\text{P}} + \hat{A}\Delta\hat{\psi}^{\text{P}}$ and integrating by parts, we can rewrite the integrals as, for example,

$$\begin{aligned} & \int_r^{\infty} dr' \Phi_{\text{top}}^{-1} \hat{D}\Delta\hat{\psi}^{\text{P}} \\ & = \int_r^{\infty} dr' \left(-\frac{d}{dr} \Phi_{\text{top}}^{-1} + \Phi_{\text{top}}^{-1} \hat{A} \right) \Delta\hat{\psi}^{\text{P}} \\ & \quad + \Phi_{\text{top}}^{-1} \Delta\hat{\psi}^{\text{P}} \Big|_r^{\infty}. \end{aligned} \quad (138)$$

It is straightforward to establish that

$$\frac{d}{dr}\Phi^{-1} - \Phi^{-1}\hat{A} = 0, \quad (139)$$

starting from $\frac{d}{dr}(\Phi^{-1}\Phi) = 0$ and using Eq. (116). This simplifies the above result to

$$\int_r^\infty dr' \Phi_{\text{top}}^{-1} \hat{D} \Delta \hat{\psi}^{\mathcal{P}} = \Phi_{\text{top}}^{-1} \Delta \hat{\psi}^{\mathcal{P}} \Big|_r^\infty. \quad (140)$$

Similarly evaluating the second integral in Eq. (137), we obtain

$$\begin{aligned} \Delta \hat{\psi}^{\mathcal{R}} &= -\Delta \hat{\psi}^{\mathcal{P}} + \Phi_- \lim_{r \rightarrow \infty} \left(\Phi_{\text{top}}^{-1} \Delta \hat{\psi}^{\mathcal{P}} \right) \\ &\quad + \Phi_+ \lim_{r \rightarrow 2M} \left(\Phi_{\text{bot}}^{-1} \Delta \hat{\psi}^{\mathcal{P}} \right). \end{aligned} \quad (141)$$

We see that the change in the puncture is counterbalanced by the change in the residual field, and the retarded integral recovers the correct result, if⁸

$$\lim_{r \rightarrow \infty} \left(\Phi_{\text{top}}^{-1} \Delta \hat{\psi}^{\mathcal{P}} \right) = 0 \quad (143)$$

and

$$\lim_{r \rightarrow 2M} \left(\Phi_{\text{bot}}^{-1} \Delta \hat{\psi}^{\mathcal{P}} \right) = 0. \quad (144)$$

We can also write this as

$$\lim_{r \rightarrow \infty} \left[\Phi_{\text{top}}^{-1} (\hat{\psi}^{\mathcal{P}} - \hat{\psi}^{\mathcal{S}}) \right] = 0 \quad (145)$$

and

$$\lim_{r \rightarrow 2M} \left[\Phi_{\text{bot}}^{-1} (\hat{\psi}^{\mathcal{P}} - \hat{\psi}^{\mathcal{S}}) \right] = 0. \quad (146)$$

These conditions dictate the required order of a puncture. For example, if we work with a puncture that includes terms up to order $(r - 2M)^n$ near the horizon, then Eq. (146) tells us that n must be large enough to ensure $\lim_{r \rightarrow 2M} [\Phi_{\text{bot}}^{-1} (r - 2M)^{n+1}] = 0$.

Equations (143) and (144) also tell us the conditions under which we actually need a puncture. If we choose

⁸ The same calculation also shows that the retarded integral yields the correct residual field if we change the puncture by a homogeneous solution near the boundaries, as in $\Delta \psi_{\pm}^{\mathcal{P}} = \Phi_{\pm} b_{\pm} \mathcal{W}_{\pm}$ for constant d -vectors b_{\pm} . Equation (141) in that case reads

$$\begin{aligned} \Delta \hat{\psi}^{\mathcal{R}} &= -\Delta \hat{\psi}^{\mathcal{P}} + \Phi_- \lim_{r \rightarrow \infty} \left(\Phi_{\text{top}}^{-1} \Phi_+ \right) b_+ \\ &\quad + \Phi_+ \lim_{r \rightarrow 2M} \left(\Phi_{\text{bot}}^{-1} \Phi_- \right) b_-. \end{aligned} \quad (142)$$

It follows from $\Phi^{-1}\Phi = \mathbf{1}_{2d \times 2d}$ that $\Phi_{\text{top}}^{-1}\Phi_+ = 0 = \Phi_{\text{bot}}^{-1}\Phi_-$, and so $\Delta \hat{\psi}^{\mathcal{R}} = -\Delta \hat{\psi}^{\mathcal{P}}$. This simply trades the homogeneous solution between the puncture and the residual field, without altering the total, physical field. Equivalently, this trades a homogeneous solution between the two terms in the boundary conditions (128).

$\Delta \hat{\psi}^{\mathcal{P}} = -\hat{\psi}^{\mathcal{P}\text{exact}}$, then $\hat{\psi}^{\mathcal{P}} = 0$ and the residual field becomes simply the retarded integral of the physical source, $\hat{\psi}^{\mathcal{R}} = -\Phi_- \int_r^\infty dr' \Phi_{\text{top}}^{-1} \hat{J} + \Phi_+ \int_{2M}^r dr' \Phi_{\text{bot}}^{-1} \hat{J}$. Equations (143) and (144) become

$$\lim_{r \rightarrow \infty} \left(\Phi_{\text{top}}^{-1} \hat{\psi}^{\mathcal{S}} \right) = 0 \quad \text{and} \quad \lim_{r \rightarrow 2M} \left(\Phi_{\text{bot}}^{-1} \hat{\psi}^{\mathcal{S}} \right) = 0. \quad (147)$$

If the conditions (147) are satisfied, then

$$\begin{aligned} \hat{\psi}^{\mathcal{R}\text{exact}} &= -\hat{\psi}^{\mathcal{P}\text{exact}} - \Phi_- \int_r^\infty dr' \Phi_{\text{top}}^{-1} \hat{J} \\ &\quad + \Phi_+ \int_{2M}^r dr' \Phi_{\text{bot}}^{-1} \hat{J}. \end{aligned} \quad (148)$$

This implies that no puncture is required: with or without a puncture, the total field $\hat{\psi}^{\mathcal{R}} + \hat{\psi}^{\mathcal{P}}$ is simply the retarded integral of the original source \hat{J} , meaning that this retarded integral automatically satisfies the correct boundary conditions. Conversely, if the conditions (147) are not satisfied, meaning

$$\lim_{r \rightarrow \infty} \left(\Phi_{\text{top}}^{-1} \hat{\psi}^{\mathcal{S}} \right) \neq 0 \quad \text{or} \quad \lim_{r \rightarrow 2M} \left(\Phi_{\text{bot}}^{-1} \hat{\psi}^{\mathcal{S}} \right) \neq 0, \quad (149)$$

then a puncture *is* required.

In summary, for a given particular solution $\hat{\psi}^{\mathcal{S}}$ in the boundary conditions (128), the retarded integral (131) yields a correct residual field so long as $\hat{\psi}^{\mathcal{S}} - \hat{\psi}^{\mathcal{P}}$ satisfies the conditions (145) and (146). We emphasise that those conditions are stronger than simply ensuring convergence of the retarded integral; two different punctures can both lead to convergent retarded integrals even if the difference between them violates (143) or (144), but in that case they will lead to two different total solutions $\hat{\psi}^{\mathcal{P}} + \hat{\psi}^{\mathcal{R}}$, satisfying different physical boundary conditions.

VI. WORLDTUBE PUNCTURE SCHEME

We now introduce our worldtube scheme. We split the domain into five regions: a near-horizon region $\Gamma_H = (2M, r_H)$, a non-punctured region $\Gamma_L = (r_H, r_L)$ (where ‘L’ stands for ‘left’), a worldtube⁹ around the particle, $\Gamma_p = (r_L, r_R)$ (where ‘R’ stands for ‘right’), another non-punctured region $\Gamma_R = (r_R, r_\infty)$, and an asymptotic region $\Gamma_\infty = (r_\infty, \infty)$. These are illustrated in Fig. 2. We assume there is a puncture at the particle, $\hat{\psi}_p^{\mathcal{P}}$, in Γ_p ; a puncture at the horizon, $\hat{\psi}_H^{\mathcal{P}}$, in Γ_H , and one at infinity, $\hat{\psi}_\infty^{\mathcal{P}}$, in Γ_∞ . We also allow the operator \hat{D} to be different in the different regions, as it will be if we use different

⁹ In three-dimensional space, each of the regions is a shell surrounding the large black hole, but we adopt traditional nomenclature by referring to the shell containing the particle as a worldtube.

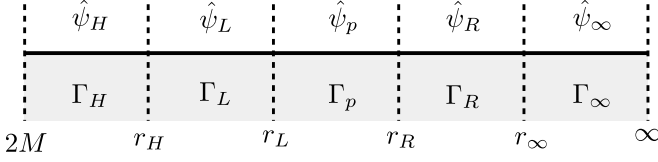


FIG. 2. Division of the numerical domain into regions Γ_H , Γ_L , Γ_p , Γ_R , and Γ_∞ . In each region Γ_a , $a \in \{H, L, p, R, \infty\}$, we use a corresponding field variable $\hat{\psi}_a$.

slicings in the different regions. We will ultimately obtain the solutions in all the regions by imposing junction conditions at the region boundaries.

In many concrete calculations we omit one or both of the regions Γ_L and Γ_R . However, for generality, we include all five regions in our description here.

Like in the preceding section, we keep our treatment generic, such that it applies both to eccentric and quasi-circular orbits.

A. General framework

In each region we define the field variable $\hat{\psi}_a$, with $a \in \{H, L, p, R, \infty\}$, as

$$\hat{\psi}_H = \hat{\psi}_H^{\text{ret}} - \hat{\psi}_H^{\mathcal{P}}, \quad (150a)$$

$$\hat{\psi}_L = \hat{\psi}_L^{\text{ret}}, \quad (150b)$$

$$\hat{\psi}_p = \hat{\psi}_p^{\text{ret}} - \hat{\psi}_p^{\mathcal{P}}, \quad (150c)$$

$$\hat{\psi}_R = \hat{\psi}_R^{\text{ret}}, \quad (150d)$$

$$\hat{\psi}_\infty = \hat{\psi}_\infty^{\text{ret}} - \hat{\psi}_\infty^{\mathcal{P}}, \quad (150e)$$

where the domain of $\hat{\psi}_a$ is Γ_a . These fields satisfy the equations

$$\hat{\mathcal{D}}_a \hat{\psi}_a := \partial_r \hat{\psi}_a + \hat{A}_a \hat{\psi}_a = \hat{J}_a^{\text{eff}}, \quad (151)$$

where \hat{A}_a is in general different in each region, and the sources are $\hat{J}_H^{\text{eff}} = \hat{J}_H - \hat{\mathcal{D}}_H \hat{\psi}_H^{\mathcal{P}}$, $\hat{J}_L^{\text{eff}} = \hat{J}_L$, $\hat{J}_p^{\text{eff}} = \hat{J}_p - \hat{\mathcal{D}}_p \hat{\psi}_p^{\mathcal{P}}$, $\hat{J}_R^{\text{eff}} = \hat{J}_R$, and $\hat{J}_\infty^{\text{eff}} = \hat{J}_\infty - \hat{\mathcal{D}}_\infty \hat{\psi}_\infty^{\mathcal{P}}$, where the raw sources \hat{J}_a are allowed to differ between regions.

The general solution in each region is

$$\hat{\psi}_a = \Phi_a \left(\int_{r_a}^r \Phi_a^{-1} \hat{J}_a^{\text{eff}} dr + a_a \right), \quad (152)$$

where $r_a \in \{2M, r_H, r_L, r_R, r_\infty\}$ is the left boundary of the domain Γ_a of $\hat{\psi}_a$. Φ_a is the matrix of homogeneous solutions to each equation with an analogous form to (115), satisfying $\partial_r \Phi_a + \hat{A}_a \Phi_a = 0$. We assume that both these homogeneous solutions and the retarded solutions

are related via transformations of the form

$$\Phi_L = T_L \Phi_H, \quad (153a)$$

$$\Phi_p = T_p \Phi_L, \quad (153b)$$

$$\Phi_R = T_R \Phi_p, \quad (153c)$$

$$\Phi_\infty = T_\infty \Phi_R, \quad (153d)$$

and analogously, $\hat{\psi}_L^{\text{ret}} = T_L \hat{\psi}_H^{\text{ret}}$, $\hat{\psi}_p^{\text{ret}} = T_p \hat{\psi}_L^{\text{ret}}$, etc. This will be the case for transformations between time slicings for the first-order field and the second-order field $\psi^{(2,0)}$ sourced by $G_{\mu\nu}^{(2,0)}$. We discuss other cases in Secs. VII and VIII. Section VIII, in particular, shows how junction conditions for second-order fields are derived from how the fields transform between slicings.

We now fix the constants in the general solution by imposing junction conditions and boundary conditions. From Eqs. (150) and (153), it follows that the junction conditions are

$$\hat{\psi}_L(r_H) = T_L \left(\hat{\psi}_H + \hat{\psi}_H^{\mathcal{P}} \right) \Big|_{r_H}, \quad (154a)$$

$$\hat{\psi}_p(r_L) = \left(T_p \hat{\psi}_L - \hat{\psi}_p^{\mathcal{P}} \right) \Big|_{r_L}, \quad (154b)$$

$$\hat{\psi}_R(r_R) = T_R \left(\hat{\psi}_p + \hat{\psi}_p^{\mathcal{P}} \right) \Big|_{r_R}, \quad (154c)$$

$$\hat{\psi}_\infty(r_\infty) = \left(T_\infty \hat{\psi}_R - \hat{\psi}_\infty^{\mathcal{P}} \right) \Big|_{r_\infty}. \quad (154d)$$

We assume boundary conditions of the form (128),

$$\hat{\psi}^{\text{ret}} = \begin{cases} \hat{\psi}_\infty^{\text{S}} + \Phi_{\infty+c_+} & \text{for } r \rightarrow \infty, \\ \hat{\psi}_H^{\text{S}} + \Phi_{H-c_-} & \text{for } r \rightarrow 2M, \end{cases} \quad (155)$$

for some constant d -vectors c_\pm , where

$$\hat{\mathcal{D}} \hat{\psi}_a^{\text{S}} = \hat{J}_a. \quad (156)$$

We also assume that the punctures $\hat{\psi}_H$ and $\hat{\psi}_\infty$ satisfy the analogues of (145) and (146):

$$\lim_{r \rightarrow \infty} \left[\Phi_{\infty\text{top}}^{-1} (\hat{\psi}_\infty^{\mathcal{P}} - \hat{\psi}_\infty^{\text{S}}) \right] = 0 \quad (157)$$

and

$$\lim_{r \rightarrow 2M} \left[\Phi_{H\text{bot}}^{-1} (\hat{\psi}_H^{\mathcal{P}} - \hat{\psi}_H^{\text{S}}) \right] = 0. \quad (158)$$

We can then impose retarded boundary conditions on $\hat{\psi}_H$ at $r = 2M$ and on $\hat{\psi}_\infty$ at $r \rightarrow \infty$, which fixes the constants in the outermost regions to be

$$a_H = (a_1^H, \dots, a_k^H, \mathbf{0}_d)^T, \quad (159)$$

$$a_\infty = \left(- \int_{r_\infty}^\infty \Phi_\infty^{-1} \hat{J}_\infty^{\text{eff}} dr, a_1^\infty, \dots, a_k^\infty \right)^T. \quad (160)$$

By combining Eqs. (153) and (154), we derive the jump conditions

$$a_L - a_H = \int_{2M}^{r_H} dr \Phi_H^{-1} \hat{J}_H^{\text{eff}} + C^H, \quad (161a)$$

$$a_p - a_L = \int_{r_H}^{r_L} dr \Phi_L^{-1} \hat{J}_L + C^L, \quad (161b)$$

$$a_R - a_p = \int_{r_L}^{r_R} dr \Phi_p^{-1} \hat{J}_p^{\text{eff}} + C^R, \quad (161c)$$

$$a_\infty - a_R = \int_{r_R}^{r_\infty} dr \Phi_R^{-1} \hat{J}_R + C^\infty, \quad (161d)$$

where

$$C^H = \Phi_H^{-1} \hat{\psi}_H^{\mathcal{P}} \Big|_{r_H}, \quad (162a)$$

$$C^L = -\Phi_L^{-1} T_p^{-1} \hat{\psi}_p^{\mathcal{P}} \Big|_{r_L}, \quad (162b)$$

$$C^R = \Phi_p^{-1} \hat{\psi}_p^{\mathcal{P}} \Big|_{r_R}, \quad (162c)$$

$$C^\infty = -\Phi_R^{-1} T_\infty^{-1} \hat{\psi}_\infty^{\mathcal{P}} \Big|_{r_\infty}. \quad (162d)$$

The boundary and jump conditions provide enough equations to determine the a_a 's. We find that

$$a_H = \left(-\int_{2M}^{\infty} dr \Phi_{\text{top}}^{-1} \hat{J}^{\text{eff}} \right) + \left(-C_{\text{top}}^H - C_{\text{top}}^L - C_{\text{top}}^R - C_{\text{top}}^\infty \right), \quad (163a)$$

$$a_L = \left(-\int_{r_H}^{\infty} dr \Phi_{\text{top}}^{-1} \hat{J}^{\text{eff}} \right) + \left(-C_{\text{top}}^L - C_{\text{top}}^R - C_{\text{top}}^\infty \right), \quad (163b)$$

$$a_p = \left(-\int_{r_L}^{\infty} dr \Phi_{\text{top}}^{-1} \hat{J}^{\text{eff}} \right) + \left(-C_{\text{top}}^R - C_{\text{top}}^\infty \right), \quad (163c)$$

$$a_R = \left(-\int_{r_R}^{\infty} dr \Phi_{\text{top}}^{-1} \hat{J}^{\text{eff}} \right) + \left(C_{\text{bot}}^H + C_{\text{bot}}^L + C_{\text{bot}}^R \right), \quad (163d)$$

$$a_\infty = \left(-\int_{r_\infty}^{\infty} dr \Phi_{\text{top}}^{-1} \hat{J}^{\text{eff}} \right) + \left(C_{\text{bot}}^H + C_{\text{bot}}^L + C_{\text{bot}}^R + C_{\text{bot}}^\infty \right), \quad (163e)$$

where we have defined $\Phi(r) := \Phi_a(r)$ for $r \in \Gamma_a$ and $\hat{J}^{\text{eff}}(r) := \hat{J}_a^{\text{eff}}(r)$ for $r \in \Gamma_a$.

With Eq. (152), Eq. (163) gives the global solution:

$$\hat{\psi} = \Phi \left[\mathbf{v} - \begin{pmatrix} C_{\text{top}}^H + C_{\text{top}}^L + C_{\text{top}}^R + C_{\text{top}}^\infty \\ \mathbf{0}_d \end{pmatrix} + C^H \theta(r - r_H) + C^L \theta(r - r_L) + C^R \theta(r - r_R) + C^\infty \theta(r - r_\infty) \right], \quad (164)$$

where \mathbf{v} is given by Eq. (125) with the replacement $\hat{J} \rightarrow \hat{J}^{\text{eff}}$, and where, following the convention just above, we have defined $\Phi(r) := \Phi_a(r)$ and $\hat{\psi}(r) := \hat{\psi}_a(r)$ for $r \in \Gamma_a$.

Equation (164) with Eqs. (125) and (162) give the solution in each region Γ_a in a form close to that of Eq. (124), but with the junction conditions across region boundaries accounted for by the additive constants C^a . In the next two sections, we describe two specific examples of this general framework.

B. Example 1: t slicing

We first consider calculations on constant- t slices (i.e., $H = 0$), with punctures allowed at the horizon, at the particle, and at infinity.

In this case, the operators \hat{D}_a are the same for all regions, equal to $\hat{D}_{[t]} = \mathbf{1}_{2d \times 2d} \frac{d}{dr} + \hat{A}_{[t]}$, where $\hat{A}_{[t]}$, defined in Eq. (71), is given by (73) (Lorenz) or (106) (Teukolsky) with $H = 0$. The matrices Φ_a are also all the same, equal to $\Phi_{[t]}$, the matrix of homogeneous solutions satisfying $\hat{D}_{[t]} \hat{\psi}_{k\pm}^{[t]} = 0$ subject to the boundary conditions (B1) and (B2) with $k(r^*) = 0$.

The solution is hence given by Eq. (164) with $\Phi = \Phi_{[t]}$ and \hat{D} (which appears in \hat{J}^{eff}) given by $\hat{D}_{[t]}$. The constants C^s are given by Eq. (162) with $T_p = T_L = T_R = T_\infty = \mathbf{1}_{2d \times 2d}$.

C. Example 2: sharp v - t - u slicing

Next we consider a sharp hyperboloidal slicing of the type described in Sec. IIB, with the sharp transitions occurring at boundaries between regions.

As an example, we consider using $s = v$ in Γ_H ; $s = t$ in Γ_L , Γ_R , and Γ_p ; and $s = u$ in Γ_∞ . The operators \hat{D}_a in this case are $\hat{D}_H = \hat{D}_{[v]}$, $\hat{D}_L = \hat{D}_R = \hat{D}_p = \hat{D}_{[t]}$, and $\hat{D}_\infty = \hat{D}_{[u]}$. Here $\hat{D}_{[s]} = \mathbf{1}_{2d \times 2d} \frac{d}{dr} + \hat{A}_{[s]}$ ($s = t, v$, or u) with $\hat{A}_{[s]}$ given by Eqs. (71) and (73) with $H = -1$ ($s = v$), $H = 0$ ($s = t$), or $H = +1$ ($s = u$). Similarly, the matrices of homogeneous solutions in this case are $\Phi_H = \Phi_{[v]}$, $\Phi_L = \Phi_R = \Phi_p = \Phi_{[t]}$, and $\Phi_\infty = \Phi_{[u]}$, and are constructed from the homogeneous solutions satisfying $\hat{D}_{[s]} \hat{\psi}_{k\pm}^{[s]} = 0$ subject to the boundary conditions (B1), (B2), or (B3) with the corresponding choice of height function $k(r^*)$.

Referring to the discussion around Eq. (84), we find that the homogeneous solutions in the different regions are related as

$$\Phi_{[v]} = P_- \Phi_{[t]}, \quad \Phi_{[u]} = P_+ \Phi_{[t]}, \quad (165a)$$

$$\Phi_{[t]} = P_+ \Phi_{[v]}, \quad \Phi_{[t]} = P_- \Phi_{[u]}, \quad (165b)$$

where

$$P_{\pm} = e^{\mp i\omega r^*} \begin{pmatrix} \mathbf{1}_{d \times d} & \mathbf{0}_{d \times d} \\ \mp i\omega f^{-1} \mathbf{1}_{d \times d} & \mathbf{1}_{d \times d} \end{pmatrix}. \quad (166)$$

Note that $P_{\pm}^{-1} = P_{\mp}$. The transformation matrices in Eq. (153) are therefore $T_L = T_{\infty} = P_+$ and $T_p = T_R = \mathbf{1}_{2d \times 2d}$.

The solution in each region is given by Eq. (164) with Φ and \hat{D} as described above. Equations (162) become

$$C^H = \Phi_{[v]}^{-1} \hat{\psi}_H^{\mathcal{P}} \Big|_{r_H}, \quad (167a)$$

$$C^L = -\Phi_{[t]}^{-1} \hat{\psi}_p^{\mathcal{P}} \Big|_{r_L}, \quad (167b)$$

$$C^R = \Phi_{[t]}^{-1} \hat{\psi}_p^{\mathcal{P}} \Big|_{r_R}, \quad (167c)$$

$$C^{\infty} = -\Phi_{[u]}^{-1} \hat{\psi}_{\infty}^{\mathcal{P}} \Big|_{r_{\infty}}, \quad (167d)$$

where the inverse matrices are evaluated at the relevant boundary between regions.

VII. DERIVATIVE OF THE FIELD WITH RESPECT TO AN ORBITAL PARAMETER

As discussed in Sec. II B, one of the required ingredients in the multiscale expansion is the parametric derivative $\bar{\partial}_{\mathcal{V}} h_{\mu\nu}^{(1)}$, where $\bar{\partial}_{\mathcal{V}}$ is defined in Eq. (32) for quasi-circular orbits and Eq. (45) for eccentric orbits. This has two types of essential input: derivatives with respect to orbital parameters p^i , and derivatives with respect to black hole parameters δM_A . Here we will only consider the first type. The second type is trivial because the contribution to $h_{\mu\nu}^{(1)}$ from δM and δJ are simple analytical functions [9], while the dependence of $h_{\mu\nu}^{(1)}$ on orbital parameters is (in general) only known numerically.

We keep our discussion in this section generic by writing a derivative of ψ with respect to an orbital parameter as $\delta\psi$. However, our treatment is slightly less generic than in the previous two sections: we assume that ψ has a compact source bounded between some minimum and maximum radius, as is the case at first order for bound orbits. ψ is then given by a retarded solution (124) that reduces to the form (120) outside the source region.

As shown in Ref. [36], the most efficient way to calculate $\delta\psi$ is to formulate a field equation for it. As we explain in this section, that field equation can be solved using the puncture scheme developed in the previous two sections. However, new junction conditions must be introduced at the boundaries between regions, and punctures must often be introduced at the outer boundaries.

A. Smooth slicing and windowed punctures

To introduce the structure of the problem, we return to the case of smooth slicing and windowed punctures. Using the same notation as in previous sections, we assume that \hat{A}, \hat{J} are functions of both r and p^i , $\hat{A} = \hat{A}(r, p^i)$ and $\hat{J} = \hat{J}(r, p^i)$. As a result, the matrix of homogeneous solutions Φ will also depend on p^i , $\Phi = \Phi(r, p^i)$.

$\hat{\psi}$ satisfies Eq. (114). By differentiating that equation with respect to an orbital parameter, we obtain a field equation for $\delta\hat{\psi}$,

$$\hat{D}\hat{\varphi} = \hat{K}, \quad (168)$$

where we have defined the field variable

$$\hat{\varphi} := \delta\hat{\psi} \quad (169)$$

and the source

$$\hat{K} = -\delta\hat{A}\hat{\psi} + \delta\hat{J}. \quad (170)$$

We note that \hat{A} only depends on p^i through a dependence on $\omega(p^i)$, meaning

$$\delta\hat{A} = 0 \quad \text{for } \omega = 0. \quad (171)$$

Equation (168) for $\hat{\varphi}$ has the same form as Eq. (114), just with a different source. However, the source is now always noncompact, due to the term $\delta\hat{A}\hat{\psi}$. Hence, in general the retarded integral may not yield the correct solution (or indeed, even converge); we will in fact find that is the case if we use t as our time function. To allow for that possibility, we introduce punctures at the boundaries, $\delta\hat{\psi}_H^{\mathcal{P}}$ and $\delta\hat{\psi}_{\infty}^{\mathcal{P}}$. For now we take these punctures to include windows, making them go to zero at some distance from the boundaries, and we define the total puncture $\delta\hat{\psi}^{\mathcal{P}} = \delta\hat{\psi}_H^{\mathcal{P}} + \delta\hat{\psi}_{\infty}^{\mathcal{P}}$. We then have

$$\hat{D}\hat{\varphi}^{\mathcal{R}} = \hat{K} - \hat{D}\hat{\varphi}^{\mathcal{P}} =: \hat{K}^{\text{eff}}. \quad (172)$$

We can now solve for $\hat{\varphi}^{\mathcal{R}}$ using the same methods we used to solve (114). The retarded integral of Eq. (172) can be read off Eq. (124) by substituting \hat{K}^{eff} for \hat{J} , yielding

$$\hat{\varphi}^{\mathcal{R}} = \Phi \mathbf{v}_{\varphi}, \quad (173)$$

where \mathbf{v}_{φ} is given by Eq. (125) with the replacement $\hat{J} \rightarrow \hat{K}^{\text{eff}}$:

$$\mathbf{v}_{\varphi} = \left(-\int_r^{\infty} dr' \Phi_{\text{top}}^{-1} \hat{K}^{\text{eff}}, \int_{2M}^r dr' \Phi_{\text{bot}}^{-1} \hat{K}^{\text{eff}} \right)^T. \quad (174)$$

It will be useful to write this as

$$\mathbf{v}_{\varphi} = \mathbf{v}_1 + \mathbf{v}_2 \quad (175)$$

with \mathbf{v}_1 and \mathbf{v}_2 given by

$$\mathbf{v}_1 = \begin{pmatrix} \int_r^\infty dr' \Phi_{\text{top}}^{-1} (\delta \hat{A} \hat{\psi} + \hat{D} \hat{\phi}^{\mathcal{P}}) \\ - \int_{2M}^r dr' \Phi_{\text{bot}}^{-1} (\delta \hat{A} \hat{\psi} + \hat{D} \hat{\phi}^{\mathcal{P}}) \end{pmatrix}, \quad (176)$$

$$\mathbf{v}_2 = \begin{pmatrix} - \int_r^\infty dr' \Phi_{\text{top}}^{-1} \delta \hat{J} \\ \int_{2M}^r dr' \Phi_{\text{bot}}^{-1} \delta \hat{J} \end{pmatrix}. \quad (177)$$

B. Worldtube method

We can reformulate the calculation of $\hat{\phi}$ in precisely the same way we did the calculation of $\hat{\psi}$ in Sec. VI. In place of Eq. (172), we have equations in each region Γ_a :

$$\hat{D}_a \hat{\phi}_a = \hat{J}_a^{\text{eff}}. \quad (178)$$

The field variable $\hat{\phi}_a$ in Γ_a can be either the physical field $\delta \hat{\psi}^{\text{ret}}$ or a residual field $\delta \hat{\psi}^{\text{ret}} - \hat{\phi}^{\mathcal{P}}$.

The general solution to this equation in each region is

$$\hat{\phi}_a = \Phi_a \left(\int_{r_a}^r \Phi_a^{-1} \hat{K}_a^{\text{eff}} dr + b_a \right). \quad (179)$$

We can find the constants b_a from junction conditions and boundary conditions, in the same manner we found the a_a 's in Sec. VI.

We readily derive the junction conditions for $\hat{\phi}$ by taking a parametric derivative of the conditions $\hat{\psi}_L^{\text{ret}}(r_H) = T_L \hat{\psi}_H^{\text{ret}}(r_H)$, $\hat{\psi}_p^{\text{ret}}(r_L) = T_p \hat{\psi}_L^{\text{ret}}(r_L)$, $\hat{\psi}_R^{\text{ret}}(r_R) = T_R \hat{\psi}_p^{\text{ret}}(r_R)$, and $\hat{\psi}_\infty^{\text{ret}}(r_\infty) = T_\infty \hat{\psi}_R^{\text{ret}}(r_\infty)$. The results are

$$\hat{\phi}_L(r_H) = \left[T_L (\hat{\phi}_H + \hat{\phi}_H^{\mathcal{P}}) + \delta T_L \hat{\psi}_H^{\text{ret}} \right]_{r_H}, \quad (180a)$$

$$\hat{\phi}_p(r_L) = \left[T_p \hat{\phi}_L + \delta T_p \hat{\psi}_L - \hat{\phi}_p^{\mathcal{P}} \right]_{r_L}, \quad (180b)$$

$$\hat{\phi}_R(r_R) = \left[T_R (\hat{\phi}_p + \hat{\phi}_p^{\mathcal{P}}) + \delta T_R \hat{\psi}_p^{\text{ret}} \right]_{r_R}, \quad (180c)$$

$$\hat{\phi}_\infty(r_\infty) = \left[T_\infty \hat{\phi}_R + \delta T_\infty \hat{\psi}_R - \hat{\phi}_\infty^{\mathcal{P}} \right]_{r_\infty}. \quad (180d)$$

Using these conditions to derive the analogues of (161), and imposing retarded boundary conditions, we obtain enough equations to fix the b_a 's. The result is that b_a is identical to a_a , as given in Eq. (163), with the replacements $\hat{J}^{\text{eff}} \rightarrow \hat{K}^{\text{eff}}$ and $C^a \rightarrow D^a$, where

$$D^H = \left[\Phi_H^{-1} \hat{\phi}_H^{\mathcal{P}} + \Phi_H^{-1} T_L^{-1} \delta T_L \hat{\psi}_H^{\text{ret}} \right]_{r_H}, \quad (181a)$$

$$D^L = \left[-\Phi_L^{-1} T_p^{-1} \hat{\phi}_p^{\mathcal{P}} + \Phi_L^{-1} T_p^{-1} \delta T_p \hat{\psi}_L \right]_{r_L}, \quad (181b)$$

$$D^R = \left[\Phi_p^{-1} \hat{\phi}_p^{\mathcal{P}} + \Phi_p^{-1} T_R^{-1} \delta T_R \hat{\psi}_p^{\text{ret}} \right]_{r_R}, \quad (181c)$$

$$D^\infty = \left[-\Phi_R^{-1} T_\infty^{-1} \hat{\phi}_\infty^{\mathcal{P}} + \Phi_R^{-1} T_\infty^{-1} \delta T_\infty \hat{\psi}_R \right]_{r_\infty}. \quad (181d)$$

Substituting the b_a 's into Eq. (179), we obtain

$$\hat{\phi} = \Phi \left[\mathbf{v}_\varphi - \begin{pmatrix} D_{\text{top}}^H + D_{\text{top}}^L + D_{\text{top}}^R + D_{\text{top}}^\infty \\ \mathbf{0}_d \end{pmatrix} + D^H \theta(r - r_H) + D^L \theta(r - r_L) + D^R \theta(r - r_R) + D^\infty \theta(r - r_\infty) \right], \quad (182)$$

with \mathbf{v}_φ given by Eq. (175). As in Eq. (164), we have defined $\hat{\phi}(r) = \hat{\phi}_a(r)$, $\Phi(r) = \Phi_a(r)$, $\hat{K}^{\text{eff}}(r) = \hat{K}_a^{\text{eff}}(r)$ for $r \in \Gamma_a$.

Equation (182) yields $\hat{\phi}$ in each region for generic slicings and punctures. We next consider the more specific cases of t slicing and sharp v - t - u slicing.

C. Example 1: t slicing

First we specialize to t slicing. As we shall see, punctures are required at the boundaries in this case.

\hat{D}_a and Φ_a are the same for all regions, which means the transformation matrices are all $T_a = 1$. We leave punctures at the horizon and infinity, but we use a point source at the particle instead of a puncture. As a result, we can combine the regions $\Gamma_L = (r_H, r_L)$, $\Gamma_p = (r_L, r_R)$, and $\Gamma_R = (r_R, r_\infty)$ into an enlarged $\Gamma_p = (r_H, r_\infty)$. With this setup, Eq. (182) reduces to

$$\hat{\phi} = \Phi_{[t]} \left[\mathbf{v}_\varphi - \begin{pmatrix} D_{\text{top}}^H + D_{\text{top}}^\infty \\ \mathbf{0}_d \end{pmatrix} + D^H \theta(r - r_H) + D^\infty \theta(r - r_\infty) \right], \quad (183)$$

where $D^\infty = -\Phi_{[t]}^{-1} \hat{\phi}_\infty^{\mathcal{P}} \Big|_{r_\infty}$ and $D^H = \Phi_{[t]}^{-1} \hat{\phi}_H^{\mathcal{P}} \Big|_{r_H}$. Again we stress that here we define $\hat{\phi}(r) = \hat{\phi}_a(r)$ for $r \in \Gamma_a$, meaning $\hat{\phi}$ is to be interpreted as $\hat{\phi}_\infty = \hat{\phi}^{\mathcal{R}}$ in Γ_∞ , for example.

To assess the need for punctures, we first analyze the integrands $\Phi_{[t]\text{top}}^{-1} \delta \hat{A}_{[t]} \hat{\psi}_{[t]}^{\text{ret}}$ and $\Phi_{[t]\text{bot}}^{-1} \delta \hat{A}_{[t]} \hat{\psi}_{[t]}^{\text{ret}}$ in Eq. (175). Our analysis appeals to the concrete form of \hat{A} in Eqs. (71), (73), and (106).

Recalling that $\delta \hat{A}_{[t]} = 0$ for $\omega = 0$ modes, we examine $\omega \neq 0$ modes at large r . We have $\delta \hat{A}_{[t]} \sim r^0$ and $\hat{\psi}_{[t]}^{\text{ret}} \sim e^{+i\omega r^*}$. $\Phi_{[t]}^{-1}$ is made up of quantities that all behave as $\sim e^{ik\omega r^*}$ for some k at large r . So in principle, $\Phi_{[t]\text{top}}^{-1} \delta \hat{A}_{[t]} \hat{\psi}_{[t]}^{\text{ret}}$ asymptotes to a sum of terms $\sim e^{ip\omega r^*}$ with different p 's. For $p = 0$, $\int_r^\infty e^{ip\omega r'^*} dr' \sim \lim_{R \rightarrow \infty} R$; for $p \neq 0$, $\int_r^\infty e^{ip\omega r'^*} dr' \sim \lim_{R \rightarrow \infty} e^{ip\omega R}$. In either case, the limit does not exist, indicating that the integral in the top row of Eq. (175) does not converge without a puncture.

For $\omega \neq 0$ modes near $r = 2M$, we have $\delta \hat{A}_{[t]} \sim f^0$ and $\hat{\psi}_{[t]}^{\text{ret}} \sim e^{-i\omega r^*}$. $\Phi_{[t]}^{-1}$ is made up of quantities that

behave as $\sim e^{iq\omega r^*}$ or $\sim f^{-1}e^{iq\omega r^*}$, for some integer q at $r \rightarrow 2M$. So in principle, $\Phi_{[t]\text{bot}}^{-1}\delta\hat{A}_{[t]}\hat{\psi}_{[t]}^{\text{ret}}$ could possess a power-law divergence at the horizon, indicating that the integral in the bottom row of Eq. (175) would diverge without a puncture.

These analytical scalings suggest the need for punctures at both the horizon and at infinity. We have confirmed this requirement numerically. We can also confirm it by considering that $\hat{\varphi}$ is a parametric derivative of a retarded field. Since $\hat{\psi}_{[t]}^{\text{ret}} \sim e^{-i\omega r^*}$ for $r \rightarrow 2M$ and $\hat{\psi}_{[t]}^{\text{ret}} \sim e^{+i\omega r^*}$ for $r \rightarrow \infty$, this implies

$$\hat{\varphi}^{\text{ret}} \sim (\delta\omega) \ln\left(\frac{r}{2M} - 1\right) e^{-i\omega r^*} \quad \text{for } r \rightarrow 2M, \quad (184)$$

$$\hat{\varphi}^{\text{ret}} \sim (\delta\omega)r^* e^{+i\omega r^*} \quad \text{for } r \rightarrow \infty. \quad (185)$$

These behaviors clearly violate the analogue of Eqs. (147), verifying the need for punctures.

We can obtain the punctures in a practical way from the large- r and near-horizon expansions (B1) or (B3). To construct the puncture at infinity, we define

$$\hat{\chi}_\infty = \Phi^{\text{out}}\mathbf{v}, \quad (186)$$

with \mathbf{v} given by Eq. (125) and

$$\Phi^{\text{out}} = \left(\mathbf{0}_{2d \times d} \mid \hat{\Psi}^{1+} \dots \hat{\Psi}^{d+} \right), \quad (187)$$

where $\hat{\Psi}^{k+} = (\Psi^{k+}, \partial_r \Psi^{k+})^T$, $k = 1, \dots, d$, and $\Psi_{\ell m}^{k+} = a_{k,0}^{\ell m}(p^i) e^{i\omega r^*}$ is the leading term in the large- r expansion (B1a). The parametric derivative is then

$$\delta\chi_\infty = \delta\Phi^{\text{out}}\mathbf{v} + \Phi^{\text{out}}\delta\mathbf{v}. \quad (188)$$

For the Lorenz-gauge case, we only need to remove the leading large- r behavior. It therefore suffices to take $\hat{\varphi}_\infty^{\mathcal{P}}$ to be the leading term in Eq. (188),

$$\hat{\varphi}_\infty^{\mathcal{P}} = i(\delta\omega)r^*\Phi^{\text{out}} \cdot \begin{pmatrix} \mathbf{0}_d \\ c_+ \end{pmatrix}, \quad (189)$$

where c_+ is given by Eq. (126). For the Teukolsky case, the general construction is the same, but three more orders must be included in the puncture to obtain a convergent retarded integral of the effective source.

The puncture at the horizon is derived analogously. We define

$$\hat{\chi}_H = \Phi^{\text{in}}\mathbf{v}, \quad (190)$$

with

$$\Phi^{\text{in}} = \left(\hat{\Psi}^{1-} \dots \hat{\Psi}^{d-} \mid \mathbf{0}_{2d \times d} \right), \quad (191)$$

where $\hat{\Psi}_{\ell m}^{k-} = (\Psi_{\ell m}^{k-}, \partial_r \Psi_{\ell m}^{k-})^T$, $k = 1, \dots, d$, and $\Psi_{\ell m}^{k-} = b_{k,0}^{\ell m}(p^i) e^{-i\omega r^*}$, the leading term in the near-horizon expansion (B1b). The parametric derivative is

$$\delta\hat{\chi}_H = \delta\Phi^{\text{in}}\mathbf{v} + \Phi^{\text{in}}\delta\mathbf{v}. \quad (192)$$

Again it suffices to include just the leading term,

$$\hat{\varphi}_H^{\mathcal{P}} = -i(\delta\omega)r^*\Phi^{\text{in}} \cdot \begin{pmatrix} c_- \\ \mathbf{0}_d \end{pmatrix}, \quad (193)$$

where c_- is given by Eq. (127).

In summary, with t slicing, the parametric derivative of the retarded field, $\delta\hat{\psi}^{\text{ret}}$, is given by

$$\delta\hat{\psi}^{\text{ret}} = \hat{\varphi}_H + \hat{\varphi}_H^{\mathcal{P}} \quad (194)$$

for $2M < r < r_H$, by

$$\delta\hat{\psi}^{\text{ret}} = \hat{\varphi}_\infty + \hat{\varphi}_\infty^{\mathcal{P}} \quad (195)$$

for $r > r_\infty$, and by

$$\delta\hat{\psi}^{\text{ret}} = \hat{\varphi}_p \quad (196)$$

for $r_H < r < r_\infty$, where $\hat{\varphi}_a$ is given by Eq. (183), with the punctures $\hat{\varphi}_\infty^{\mathcal{P}}$ and $\hat{\varphi}_H^{\mathcal{P}}$ given by Eqs. (189) and (193).

D. Example 2: v - t - u slicing

We next consider sharp v - t - u slicing. This is the slicing used in our numerical calculations of φ , and our description in this section focuses in on the particular choices we make in our numerical implementation. Unlike in previous sections, here we also divide the discussion between Lorenz-gauge and Teukolsky calculations as they differ in important ways.

Like in the case of t slicing, we do not use a puncture at the particle.

1. Lorenz Gauge

In our Lorenz-gauge calculations, we merge Γ_L and Γ_R into Γ_p . The matrices of homogeneous solutions in the three regions $\Gamma_H, \Gamma_p, \Gamma_\infty$ are $\Phi_H = \Phi_{[v]}$, $\Phi_p = \Phi_{[t]}$, and $\Phi_\infty = \Phi_{[u]}$, as described in Sec. VIC.

We show below that a puncture is not required with this setup. Equation (182) therefore reduces to

$$\hat{\varphi} = \Phi \left[\mathbf{v}_\varphi - \begin{pmatrix} D_{\text{top}}^H + D_{\text{top}}^\infty \\ \mathbf{0}_d \end{pmatrix} + D^H\theta(r - r_H) + D^\infty\theta(r - r_\infty) \right], \quad (197)$$

where $D^H = \Phi_{[v]}^{-1}P_- \delta P_+ \hat{\psi}_{[v]}^{\text{ret}}$ and $D^\infty = \Phi_{[t]}^{-1}P_- \delta P_+ \hat{\psi}_{[t]}^{\text{ret}}$. Explicitly,

$$D^H = -i\delta\omega\Phi_{[v]}^{-1} \begin{pmatrix} r^*\mathbf{1}_{d \times d} & \mathbf{0}_{d \times d} \\ f^{-1}\mathbf{1}_{d \times d} & r^*\mathbf{1}_{d \times d} \end{pmatrix} \hat{\psi}_{[v]}^{\text{ret}} \Big|_{r=r_H}, \quad (198)$$

$$D^\infty = -i\delta\omega\Phi_{[t]}^{-1} \begin{pmatrix} r^*\mathbf{1}_{d \times d} & \mathbf{0}_{d \times d} \\ f^{-1}\mathbf{1}_{d \times d} & r^*\mathbf{1}_{d \times d} \end{pmatrix} \hat{\psi}_{[t]}^{\text{ret}} \Big|_{r=r_\infty}. \quad (199)$$

To justify the conclusion that no punctures are required, we first consider the integrands that appear in Eq. (175). From the large- r behavior (B1a), we have $\hat{\psi}_{[u]}^{\text{ret}} \sim (r^0, \dots, r^0, 1/r^2, \dots, 1/r^2)^T$; the absence of the phase factor $e^{i\omega r^*}$ in u slicing means that the r derivative of the leading term vanishes, leading to the $\sim 1/r^2$ behavior in $\partial_r \hat{\psi}_{[u]}^{\text{ret}}$. We also have

$$\delta \hat{A}_{[u]} \sim \begin{pmatrix} \mathbf{0}_{d \times d} & \mathbf{0}_{d \times d} \\ r^{-2} \mathbf{1}_{d \times d} & r^0 \mathbf{1}_{d \times d} \end{pmatrix}. \quad (200)$$

Hence, the source in Γ_∞ , $\hat{K}_\infty = -\delta \hat{A}_{[u]} \hat{\psi}_{[u]}^{\text{ret}}$, behaves as $\sim r^{-2}$. To assess the falloff of the integrand $\Phi_{[u]\text{top}}^{-1} \delta \hat{A}_{[u]} \hat{\psi}_{[u]}^{\text{ret}}$, we also require the falloff of $\Phi_{[u]\text{top}}^{-1}$. From the large- r behavior (B1a), we have the block form

$$\Phi_{[u]} \sim \begin{pmatrix} (1 + e^{-2i\omega r^*}) \mathbf{1}_{d \times d} & r^0 \mathbf{1}_{d \times d} \\ e^{-2i\omega r^*} \mathbf{1}_{d \times d} & r^{-2} \mathbf{1}_{d \times d} \end{pmatrix}, \quad (201)$$

from which we can derive $\Phi_{[u]\text{top}}^{-1} \sim r^0$ (possibly with oscillatory terms). Therefore the integrand in the upper half of Eq. (175) falls off as $1/r^2$ (again, possibly with oscillatory terms), and the integrals converge without a need for a puncture.

The core of this sketch is that in hyperboloidal slicing, the outgoing modes at infinity do not contain an oscillatory factor. A similar sketch applies for the integral in the lower half of Eq. (175), using the fact that the ingoing modes at the horizon likewise contain no oscillatory factor.

We have also numerically verified that the stronger (but necessary) conditions (147) are met. The key reason is again the lack of oscillatory factors. The correct boundary conditions are provided by the parametric derivative of the retarded field $\hat{\psi}_{[vtu]}^{\text{ret}}$. Because there are no oscillatory factors in $\hat{\psi}_{[vtu]}^{\text{ret}}$, we have that $\delta \hat{\psi}_{[u]}^{\text{ret}}$ has the same falloff as $\hat{\psi}_{[u]}^{\text{ret}}$ as $r \rightarrow \infty$, and $\delta \hat{\psi}_{[v]}^{\text{ret}}$ has the same behavior as $\hat{\psi}_{[v]}^{\text{ret}}$ as $r \rightarrow 2M$; this contrasts with the behavior in t slicing, illustrated in Eqs. (188) and (192), where the parametric derivative introduces irregularities at the boundaries.

In summary, with v - t - u slicing, $\delta \hat{\psi}^{\text{ret}}$ is given by Eq. (197) with Eq. (175) and vanishing punctures in \mathbf{v}_φ .

2. Teukolsky

We now consider the equivalent calculation in our Teukolsky formalism of Sec. IV A. Similar to the Lorenz-gauge calculations, we consolidate Γ_L and Γ_R into a single region, Γ_p . But, unlike in the Lorenz gauge, it is necessary to include a puncture, $\hat{\varphi}_\infty$ in the asymptotic

regime of Γ_∞ . The solution in Eq. (182) reduces to

$$\hat{\varphi} = \Phi \left[\mathbf{v}_\varphi - \begin{pmatrix} D_{\text{top}}^H + D_{\text{top}}^\infty \\ \mathbf{0}_d \end{pmatrix} + D^H \theta(r - r_H) + D^\infty \theta(r - r_\infty) \right], \quad (202)$$

where

$$D^H = \Phi_{[v]}^{-1} P_- \delta P_+ \hat{\psi}_{[v]}^{\text{ret}} \\ D^\infty = \left[-\Phi_{[t]}^{-1} P_- \hat{\varphi}_\infty^{\mathcal{P}} + \Phi_{[t]}^{-1} P_- \delta P_+ \hat{\psi}_{[t]}^{\text{ret}} \right]_{r_\infty}, \quad (203)$$

with $\Phi_H = \Phi_{[v]}$, $\Phi_p = \Phi_{[t]}$, and $\Phi_\infty = \Phi_{[u]}$ in the regions Γ_H , Γ_p , Γ_∞ respectively. In this section we wish to demonstrate the need for an appropriate puncture within the asymptotic region Γ_∞ despite the introduction of hyperboloidal slicing.

Once more, let us consider the integrals over the extended source term that appear in Eq. (175). The boundary conditions of the homogeneous solutions to the Teukolsky equation results imply, under rescaling, $\hat{\psi}_{[u]}^{\text{ret}} \sim (r^0, 1/r^2)^T$, like in the Lorenz gauge.

In the Teukolsky form of our worldtube method, $\delta \hat{A}_{[u]}$ is given, at leading order, by

$$\delta \hat{A}_{[u]} \sim \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ r^{-2} & r^0 \end{pmatrix}. \quad (204)$$

Therefore the source behaves as $\hat{K}_\infty \sim r^{-2}$ in the asymptotic region Γ_∞ , again just as in the Lorenz gauge. However, the falloff of the entire integrand is where the similarities with the Lorenz gauge end. If we consider the final factor in the integrand, $\Phi_{[u]\text{top}}^{-1}$, we find that Eqs. (112) and (113) imply

$$\Phi_{[u]} \sim \begin{pmatrix} r^0 + r^{2s} e^{-2i\omega r^*} & r^0 \\ r^{-2} + r^{2s} e^{-2i\omega r^*} & r^{-2} \end{pmatrix}, \quad (205)$$

which leads to $\Phi_{[u]\text{top}}^{-1} \sim r^{-2s}(r^{-2}, r^0)^T$ (neglecting oscillatory factors).¹⁰ The integrands in the upper half of the solution (175) therefore diverge as $\Phi_{[u]\text{top}}^{-1} \delta \hat{A}_{[u]} \hat{\psi}_{[u]}^{\text{ret}} \sim r^{-2(s+1)}$. For the spin-weight $s = -2$ that we are considering here, $\Phi_{[u]\text{top}}^{-1} \delta \hat{A}_{[u]} \hat{\psi}_{[u]}^{\text{ret}} \sim r^2$. Hence the integrals

¹⁰ For a generic matrix of the form (205), the large- r growth of $\Phi_{[u]\text{top}}^{-1}$ is slower than our displayed scaling. Our scaling relies on the fact that the determinant of the leading-order large- r term in $\Phi_{[u]}$ vanishes. We can write that matrix as $\begin{pmatrix} ar^0 & br^0 \\ cr^{-2} & dr^{-2} \end{pmatrix}$. Each column here comes from the large- r expansion of an outgoing wave solution $[\mathbf{s}R_{\ell m}^+, \partial_r(\mathbf{s}R_{\ell m}^+)]^T$, multiplied by a constant a or b , with $\mathbf{s}R_{\ell m}^+ = r^0 + a_1 r^{-1} + \mathcal{O}(r^{-2})$ for some constant a_1 . We therefore have $c = -aa_1$ and $d = -ba_1$, which makes the determinant vanish.

diverge, and to obtain a physical solution one requires a suitable puncture in Γ_∞ .

In our Teukolsky calculation, we obtain punctures in the same manner as in Sec. VII C, by appealing to the large- r expansions in Appendix B 2. To construct a suitable puncture in Γ_∞ , we again use the definition in Eq. (186), with $\Phi^{\text{out}} = (\mathbf{0}_{2 \times 1} | \hat{\Psi}^+)$. Here $\hat{\Psi}^+$ is given by terms derived from the asymptotic expansion in Eq. (B3),

$$\Psi_{\ell m}^+ = f^{-2} \sum_{j=0}^{j_{\text{max}}} \frac{a_j^{\ell m}(p^i)}{(\omega r)^j}. \quad (206)$$

Here $j_{\text{max}} \geq 2$; since the divergence is $\sim r^2$ in the integrand, one must consider an expansion at least up to $\mathcal{O}(r^{-2})$. This is to ensure the effective source $\hat{K}_\infty^{\text{eff}}$ falls off sufficiently quickly for the integral to converge. The puncture, $\hat{\varphi}_\infty^{\mathcal{P}}$, is therefore defined by taking the first term of the parametric derivative, $\delta\chi_\infty$, in Eq. (188) with $\delta\Phi^{\text{out}}$ derived from the asymptotic expansion in Eq. (206). This yields

$$\delta\Phi^{\text{out}} = \frac{\delta\omega}{f^2 r} \sum_{j=0}^{j_{\text{max}}} j \frac{a_j^{\ell m}(p^i)}{(\omega r)^{j-1}} \begin{pmatrix} 0 & r^2 \\ 0 & -jr - 4Mf^{-1} \end{pmatrix}, \quad (207)$$

such that the final puncture is given by

$$\hat{\varphi}_\infty^{\mathcal{P}} = \delta\Phi^{\text{out}} \cdot \begin{pmatrix} 0 \\ c_+ \end{pmatrix}, \quad (208)$$

with c_+ given by Eq. (126).

VIII. FIELD EQUATIONS WITH PARAMETRIC-DERIVATIVE SOURCES

As a final case, we consider a field sourced by a parametric derivative of a lower-order field. This is the type of source in the field equation (77), which we rewrite here as

$$\hat{D}_a \hat{\psi}_a^{(1,1)} = \hat{J}_{\text{eff},a}^{(1,1)}. \quad (209)$$

We restrict our analysis to quasicircular orbits for simplicity, but the extension to eccentric orbits is immediate. For simplicity, we also assume the falloff properties of the Lorenz-gauge Φ^{-1} , but the discussion is straightforwardly extended to allow for the Teukolsky falloff behavior.

We organize our analysis somewhat differently here than in the preceding three sections. Rather than first considering a generic formulation and then examining the scheme in t slicing and in v - t - u slicing, here we begin with the fact that no punctures at the boundaries are required in v - t - u slicing (for fields exhibiting the Lorenz-gauge falloff); this follows from the scaling of the sources in u and v slicing, given in Eqs. (94) and (96), and the arguments in Sec. VII D. We then analyse the transformation between slicings in order to derive punctures in t slicing and junction conditions in v - t - u slicing. Finally, we summarize the solution in v - t - u slicing.

A. Junction conditions and punctures

We first consider the transformation from u to t slicing. We consider a field $\psi_{[u]}[\mathcal{J}_I(u)]e^{-im\phi_p(u)}$ in u slicing, suppressing the dependence on r and ε . Expanding functions of u around their values at t , we obtain

$$\phi_p(u) = \phi_p(t) - r^* \Omega(t) + \frac{\varepsilon}{2} (r^*)^2 F_\Omega^{(0)}(t) + \mathcal{O}(\varepsilon^2), \quad (210)$$

$$\mathcal{J}_I(u) = \mathcal{J}_I(t) - \varepsilon r^* F_I^{(0)}(t) + \mathcal{O}(\varepsilon^2), \quad (211)$$

and therefore

$$\begin{aligned} & \psi_{[u]}[\mathcal{J}_I(u)]e^{-im\phi_p(u)} \\ &= \left\{ \psi_{[u]}[\mathcal{J}_I(t)] - \varepsilon \left[r^* \vec{\partial}_\nu \psi_{[u]} \right. \right. \\ & \quad \left. \left. + \frac{i}{2} (r^*)^2 m F_\Omega^{(0)} \psi_{[u]} \right] + \mathcal{O}(\varepsilon^2) \right\} e^{im[\Omega r^* - \phi_p(t)]}, \end{aligned} \quad (212)$$

where all functions on the right are evaluated at time t . Equating the right-hand side of Eq. (212) to $\psi_{[t]}[\mathcal{J}_I(t)]e^{-im\phi_p(t)}$, and writing the expansions

$$\psi_{[t]} = \varepsilon \psi_{[t]}^{(1)} + \varepsilon^2 \psi_{[t]}^{(2)} + \mathcal{O}(\varepsilon^3) \quad (213)$$

and

$$\psi_{[u]} = \varepsilon \psi_{[u]}^{(1)} + \varepsilon^2 \psi_{[u]}^{(2)} + \mathcal{O}(\varepsilon^3), \quad (214)$$

we find $\psi_{[u]}^{(1)} = \psi_{[t]}^{(1)} e^{-im\Omega r^*}$ and

$$\psi_{[u]}^{(2)} = \left(\psi_{[t]}^{(2)} + \Delta \psi_{[t]}^{(2)} \right) e^{-im\Omega r^*}, \quad (215)$$

where

$$\Delta \psi_{[t]}^{(2)} = r^* \vec{\partial}_\nu \psi_{[t]}^{(1)} - \frac{i}{2} (r^*)^2 m F_\Omega^{(0)} \psi_{[t]}^{(1)}. \quad (216)$$

Here all functions are evaluated at the same values of their arguments.

We relate

$$\hat{\psi}_{[u]}^{(2)} = \left(\psi_{[u]}^{(2)}, \partial_r \psi_{[u]}^{(2)} \right)^T \quad (217)$$

to

$$\hat{\psi}_{[t]}^{(2)} = \left(\psi_{[t]}^{(2)}, \partial_r \psi_{[t]}^{(2)} \right)^T \quad (218)$$

by taking a radial derivative of Eq. (215). This yields

$$\hat{\psi}_{[u]}^{(2)} = P_+ \left(\hat{\psi}_{[t]}^{(2)} + \Delta \hat{\psi}_{[t]}^{(2)} \right), \quad (219)$$

where

$$\begin{aligned} \Delta \hat{\psi}_{[t]}^{(2)} &= r^* \vec{\partial}_\nu \hat{\psi}_{[t]}^{(1)} - \frac{i}{2} (r^*)^2 m F_\Omega^{(0)} \hat{\psi}_{[t]}^{(1)} \\ & \quad + f^{-1} \left(\mathbf{0}_a, \vec{\partial}_\nu \psi_{[t]}^{(1)} - im F_\Omega^{(0)} r^* \psi_{[t]}^{(1)} \right)^T. \end{aligned} \quad (220)$$

Noting that every term in the transformation involves a forcing function, we can also write

$$\hat{\psi}_{[u]}^{(1,1)} = P_+ \left(\hat{\psi}_{[t]}^{(1,1)} + \Delta \hat{\psi}_{[t]}^{(2)} \right), \quad (221)$$

while the rest of $\hat{\psi}^{(2)}$ transforms in the trivial way:

$$\hat{\psi}_{[u]}^{(2,0)} = P_+ \hat{\psi}_{[t]}^{(2,0)}. \quad (222)$$

Equation (221) is the junction condition at a boundary between t and u slicings. The same equation holds at a boundary between v and t slicings, with the relabeling $t \rightarrow v$, $u \rightarrow t$:

$$\hat{\psi}_{[t]}^{(1,1)} = P_+ \left(\hat{\psi}_{[v]}^{(1,1)} + \Delta \hat{\psi}_{[v]}^{(2)} \right), \quad (223)$$

where

$$\begin{aligned} \Delta \hat{\psi}_{[v]}^{(2)} &= r^* \vec{\partial}_V \hat{\psi}_{[v]}^{(1)} - \frac{i}{2} (r^*)^2 m F_\Omega^{(0)} \hat{\psi}_{[v]}^{(1)} \\ &+ f^{-1} \left(\mathbf{0}_d, \vec{\partial}_V \hat{\psi}_{[v]}^{(1)} - im F_\Omega^{(0)} r^* \hat{\psi}_{[v]}^{(1)} \right)^T. \end{aligned} \quad (224)$$

In addition to providing a junction condition, Eq. (223) can be used to construct a puncture at the horizon in t slicing. The singularity at the horizon comes from the second term, which then serves as a puncture,

$$\hat{\psi}_{H[t]}^{\mathcal{P}(1,1)} = P_+ \Delta \hat{\psi}_{[v]}^{(2)}. \quad (225)$$

A puncture at infinity can be constructed in the same way. Following the same steps that led to Eq. (221), we find

$$\hat{\psi}_{[t]}^{(1,1)} = P_- \left(\hat{\psi}_{[u]}^{(1,1)} + \Delta \hat{\psi}_{[u]}^{(2)} \right), \quad (226)$$

where

$$\begin{aligned} \Delta \hat{\psi}_{[u]}^{(2)} &= -r^* \vec{\partial}_V \hat{\psi}_{[u]}^{(1)} - \frac{i}{2} (r^*)^2 m F_\Omega^{(0)} \hat{\psi}_{[u]}^{(1)} \\ &- f^{-1} \left(\mathbf{0}_d, \vec{\partial}_V \hat{\psi}_{[u]}^{(1)} + im F_\Omega^{(0)} r^* \hat{\psi}_{[u]}^{(1)} \right)^T. \end{aligned} \quad (227)$$

A valid puncture at infinity is therefore

$$\hat{\psi}_{\infty[t]}^{\mathcal{P}(1,1)} = P_- \Delta \hat{\psi}_{[u]}^{(2)}. \quad (228)$$

B. Example: v - t - u slicing

As a concrete example, we now specialize to the following setup:

- (i) in Γ_H , we use v slicing and a puncture $\hat{\psi}_H^{\mathcal{P}}$
- (ii) in Γ_L , we use v slicing and no puncture
- (iii) in Γ_p , we use t slicing and a puncture $\hat{\psi}_p^{\mathcal{P}}$
- (iv) we omit Γ_R

(v) in Γ_∞ , we use u slicing and a puncture $\hat{\psi}_\infty^{\mathcal{P}}$.

This is the arrangement used in Refs. [7, 17, 18].

Following the same steps as in previous sections, starting from a solution of the form (152), we arrive at the first three subequations in Eq. (161) with

$$C_{(1,1)}^H = \Phi_{[v]}^{-1} \hat{\psi}_H^{\mathcal{P}(1,1)} \Big|_{r_H}, \quad (229a)$$

$$C_{(1,1)}^L = \Phi_{[t]}^{-1} \left[P_+ \Delta \hat{\psi}_{[v]}^{(2)} - \hat{\psi}_p^{\mathcal{P}(1,1)} \right] \Big|_{r_L}, \quad (229b)$$

$$C_{(1,1)}^\infty = \Phi_{[u]}^{-1} \left\{ P_+ \left[\Delta \hat{\psi}_{[t]}^{(2)} + \hat{\psi}_p^{\mathcal{P}(1,1)} \right] - \hat{\psi}_\infty^{\mathcal{P}(1,1)} \right\} \Big|_{r_\infty} \quad (229c)$$

and with the replacements $r_R = r_\infty$, $C^R \rightarrow C_{(1,1)}^\infty$, and $a_R \rightarrow a_\infty$. The solution can then be put in the form (164) with $r_R = r_\infty$ and C^R set to zero.

Here, for generality, we allow for punctures at infinity and the horizon. Though they are not needed in v - t - u slicing, they can be used to accelerate convergence of integrals.

IX. DEMONSTRATION 1: LORENZ-GAUGE CALCULATIONS FOR QUASICIRCULAR ORBITS

As a demonstration of our method, we consider the Lorenz-gauge field equations for a point mass on a quasicircular orbit. In that context, we calculate the first-order metric perturbation $\bar{h}_{i\ell m}^{(1)}$ and the parametric derivative $\partial_{r_0} \bar{h}_{i\ell m}^{(1)}$, where $r_0 = M(M\Omega)^{-2/3}$ is the leading-order orbital radius.

A. Calculation of $\bar{h}_{i\ell m}^{(1)}$

In t slicing, the field equations for $\bar{h}_{i\ell m}^{(1)}$ are identical to Ref. [49]'s Lorenz-gauge frequency-domain field equations for a particle on a circular geodesic of radius r_0 . We write them for generic slicing in matrix form as

$$\hat{\mathcal{D}}_a \hat{\psi}_a^{(1)} = \hat{\mathcal{J}}_a^{(1)}, \quad (230)$$

where $\hat{\mathcal{D}}$ is defined by Eq. (70) with Eqs. (71) and (73).

The point source takes the form

$$\hat{\mathcal{J}}^{(1)} = \hat{\mathcal{J}}^{\text{PP}}(r_0) \delta(r - r_0), \quad (231)$$

where $\hat{\mathcal{J}}^{\text{PP}} = (\mathbf{0}_d, J^{pp})^T$ and

$$J^{pp} = \beta \begin{cases} (t_1 t_3 t_5)^T & \ell > 0, m = 0, \ell \text{ even}, \\ t_8 & \ell > 0, m = 0, \ell \text{ odd}, \\ (t_1 t_3 t_5 t_6)^T & \ell = 1, m = 1, \\ (t_9 t_{10})^T & \ell, m > 0, \ell + m \text{ odd}, \\ (t_1 t_3 t_5 t_6 t_7)^T & \ell, m > 0, \ell + m \text{ even}, \end{cases} \quad (232)$$

with $\beta = 64\pi M/f_0^2$ and [48, 49]

$$t_{i\ell m}^0 = -\frac{1}{4}\mathcal{E}_0\alpha_{i\ell m} \begin{cases} Y_{\ell m}^*(\pi/2, 0) & i = 1, \dots, 7 \\ \partial_\theta Y_{\ell m}^*(\pi/2, 0) & i = 8, 9, 10. \end{cases} \quad (233)$$

Here $\mathcal{E}_0 = f_0/\sqrt{1-3M/r_0}$, with $f_0 = 1 - 2M/r_0$, is the specific energy of a point mass on a circular geodesic of radius r_0 , and the $\alpha_{i\ell m}$'s are given by (suppressing ℓm labels)

$$\alpha_1 = f_0^2/r_0, \quad \alpha_{2,5,9} = 0, \quad (234a)$$

$$\alpha_3 = f_0/r_0, \quad \alpha_4 = 2if_0m\Omega, \quad (234b)$$

$$\alpha_6 = r_0\Omega^2, \quad \alpha_7 = r_0\Omega^2[\ell(\ell+1) - 2m^2], \quad (234c)$$

$$\alpha_8 = 2f_0\Omega, \quad \alpha_{10} = 2imr_0\Omega^2. \quad (234d)$$

Note that the $i = 2, 5, 9$ equations are sourceless.

With this source, if we use a continuous slicing, we can immediately write the solution in the form (124). Equation (125) reduces to

$$\mathbf{v}^{(1)} = \mathbf{v}^- \theta(r_0 - r) + \mathbf{v}^+ \theta(r - r_0), \quad (235)$$

where

$$\mathbf{v}^- = \begin{pmatrix} -\Phi_{0\text{top}}^{-1} \hat{J}^{\text{PP}} \\ \mathbf{0}_d \end{pmatrix}, \quad \mathbf{v}^+ = \begin{pmatrix} \mathbf{0}_d \\ \Phi_{0\text{bot}}^{-1} \hat{J}^{\text{PP}} \end{pmatrix}. \quad (236)$$

Here we use $\Phi_0 := \Phi(r_0)$ for brevity. The solution (124) thus becomes

$$\hat{\psi}^{(1)} = \hat{\psi}_-^{(1)} \theta(r_0 - r) + \hat{\psi}_+^{(1)} \theta(r - r_0), \quad (237)$$

where $\hat{\psi}_\pm^{(1)} = \Phi \mathbf{v}^\pm$. This is the standard point-particle solution in, e.g., Ref. [49].

In sharp v - t - u slicing, Eq. (237) remains valid, with a simple change: in $\hat{\psi}_\pm^{(1)} = \Phi \mathbf{v}^\pm$, the matrix Φ becomes $\Phi_{[v]}$, $\Phi_{[t]}$, or $\Phi_{[u]}$, depending on the region where $\hat{\psi}_\pm^{(1)}$ is evaluated.

We evaluate this solution using the following method:

1. Fix a zeroth-order orbital radius r_0 .
2. For each ℓm mode, construct the matrix Φ of homogeneous solutions as reviewed in Appendix B 1. Φ is output and stored on a grid determined by an adaptive solver.
3. Calculate the retarded field for the column vector (72) using Eq. (237). In the calculation of $\mathbf{v}^{(1)}$, we invert the Φ matrix using the lower-upper (LU) decomposition method. Integrations and matrix inversions are performed on the same grid as in step 2.
4. For the gauge modes, we calculate the retarded field from the gauge conditions (A18). For $\ell = m = 2$, these gauge modes are $\bar{h}_2^{(1)}$ and $\bar{h}_4^{(1)}$. We found significant numerical errors in the region close to

the inner boundary r_{in} due to a loss of precision when subtracting one large number from another in the gauge conditions (A18). We used long double variables when computing these modes to resolve this issue.

We compared our results for several modes against the same computation performed in *Mathematica* to validate our code. We also compared our results for $\bar{h}_{[t]}^{(1)}$ with data from the code in Ref. [60] and found relative differences of $\lesssim 10^{-12}$, except at points near the horizon, where we found we achieved more accurate results through our use of the greater-than-machine-precision routine described in Appendix B.

In Fig. 3 we compare the $\ell = 2, m = 2$, even-parity mode of $\bar{h}_{i\ell m}^{(1)}$ with t slicing and with v - t - u slicing. The jumps in $\text{Re}(\bar{h}_{[vtu]}^{(1)})$ occur where the slicing changes from v to t or from t to u . Note that $\bar{h}_{i\ell m}^{(1)}$ on different slices can only differ by a complex phase, such that the modulus $|\bar{h}_{[vtu]}^{(1)}|$ is continuous across slices. Because v - t - u slicing follows wavefronts, $\bar{h}_{[vtu]}^{(1)}$ contains no oscillations, while $\bar{h}_{[t]}^{(1)}$ contains constant-amplitude oscillations at large r . However, the oscillations near the horizon would only become visible at points much closer to the horizon.

To compare our results for $\bar{h}_{[t]}^{(1)}$ and $\bar{h}_{[vtu]}^{(1)}$, we transform the $\bar{h}_{[t]}^{(1)}$ data onto v - t - u slices using the relationship

$$\bar{h}_{[vtu]}^{(1)} = e^{-i\omega k(r^*)} \bar{h}_{[t]}^{(1)}. \quad (238)$$

Here $k(r^*)$ is given by Eq. (18), which we restate here for convenience: $k = -r^*$ for v slicing, $k = 0$ for t slicing, and $k = +r^*$ for u slicing. After performing this transformation, we find that the results in the different slicings agree to within a relative difference of $\lesssim 10^{-12}$.

B. Calculation of $\partial_{r_0} \bar{h}_{i\ell m}^{(1)}$

1. Overview

We next consider the field $\delta\hat{\psi}^{(1)}$, where we now let

$$\delta := \partial_{r_0}. \quad (239)$$

For our quasicircular orbits, the field equation satisfied by $\hat{\varphi}^{\text{ret}} = \delta\hat{\psi}^{(1)}$ is

$$\hat{\mathcal{D}}\hat{\varphi}^{\text{ret}} = \hat{K}^{(1)}, \quad (240)$$

where the source is

$$\hat{K}^{(1)} = -\delta\hat{A}\hat{\psi}^{(1)} + \delta\hat{J}^{(1)}. \quad (241)$$

The first term in $\hat{K}^{(1)}$ is an extended source,

$$\begin{aligned} \delta\hat{A}\hat{\psi}^{(1)} &= \delta\hat{A}\hat{\psi}_-^{(1)}\theta(r_0 - r) \\ &\quad + \delta\hat{A}\hat{\psi}_+^{(1)}\theta(r - r_0), \end{aligned} \quad (242)$$

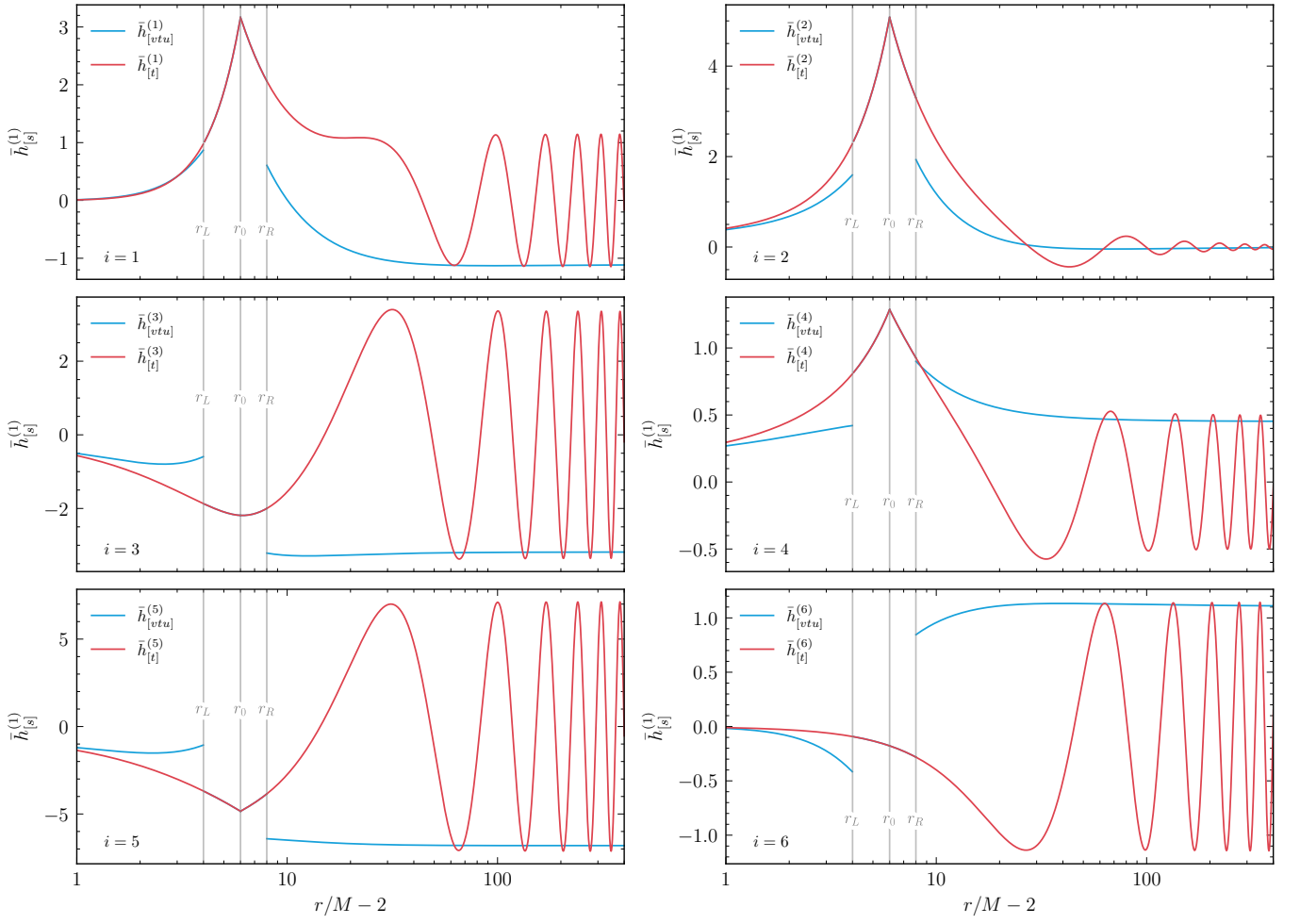


FIG. 3. $\text{Re}(\bar{h}_{[vtu]}^{(i)})$ (blue line) and $\text{Re}(\bar{h}_{[t]}^{(i)})$ (red line) for all nonvanishing i modes with $\ell = 2, m = 2, r_0 = 8M$. Note that we have not included the $i = 7$ BLS mode in this figure for brevity as this is qualitatively the same as the $i = 6$ mode.

where $\hat{\psi}_{\pm}^{(1)} = \Phi \mathbf{v}^{\pm}$ with \mathbf{v}^{\pm} as given in Eq. (236). \hat{A} is given in terms of A and B in Eq. (71), where A and B are given by (73). Taking a parametric derivative, we obtain

$$\delta \hat{A} = \begin{pmatrix} \mathbf{0}_{d \times d} & \mathbf{0}_{d \times d} \\ \delta A & \delta B \end{pmatrix}, \quad (243)$$

where

$$\begin{aligned} \delta A = & f^{-2} [2(1 - H^2) \omega_m \delta \omega_m - 2\omega_m^2 H \delta H \\ & + i\delta \omega_m H' + i\omega_m \delta H'] \mathbf{1}_{d \times d} \\ & + \delta \mathcal{M}_h, \end{aligned} \quad (244a)$$

$$\delta B = 2if^{-1} (\delta \omega_m H + \omega_m \delta H) \mathbf{1}_{d \times d}. \quad (244b)$$

Here $\delta \omega_m = m\delta\Omega = -\frac{3}{2}m\sqrt{M/r_0^5}$, and we recall the notation $H' = dH/dr^*$. $\delta \mathcal{M}_h$ is given explicitly in Eqs. (A15) and (A16). We have allowed the height function to depend on r_0 , in the case that the slicing evolves along with the orbit.

Given that $\hat{J}^{(1)} = \hat{J}^{\text{PP}}\delta(r - r_0)$, the second source term

in Eq. (241) is restricted to $r = r_0$:

$$\delta \hat{J}^{(1)} = \delta \hat{J}^{\text{PP}}\delta(r - r_0) - \hat{J}^{\text{PP}}\delta'(r - r_0). \quad (245)$$

We solve the field equation (240) for $\partial_{r_0} \bar{h}_{i\ell m}^{(1)}$ on t and v - t - u slices. In all cases, we evaluate integrals over extended sources using a Gauss-Kronrod quadrature routine.

2. $\partial_{r_0} \bar{h}_{i\ell m}^{(1)}$ on t slices

We obtain the solution for $\partial_{r_0} \bar{h}_{[t]}^{(1)}$ using Eq. (183), with punctures at the horizon and at infinity constructed according to Eqs. (189) and (193).

The main input to the solution is $\mathbf{v}_{\varphi} = \mathbf{v}_1 + \mathbf{v}_2$, where \mathbf{v}_1 and \mathbf{v}_2 are the integrals of source terms defined in Eqs. (176) and (177).

Given Eq. (242), it follows that

$$\begin{aligned} \mathbf{v}_1 &= \begin{pmatrix} I_1 + I_2 \\ -I_3 \end{pmatrix} \theta(r_0 - r) \\ &+ \begin{pmatrix} I_4 \\ -I_5 - I_6 \end{pmatrix} \theta(r - r_0), \end{aligned} \quad (246)$$

with

$$I_1 = \int_{r_0}^{\infty} dr' \Phi_{\text{top}}^{-1} \left(\delta \hat{A} \hat{\psi}_+^{\text{ret}} + \hat{\mathcal{D}} \hat{\varphi}_{\infty}^{\mathcal{P}} \right), \quad (247a)$$

$$I_2 = \int_r^{r_0} dr' \Phi_{\text{top}}^{-1} \left(\delta \hat{A} \hat{\psi}_-^{\text{ret}} + \hat{\mathcal{D}} \hat{\varphi}_H^{\mathcal{P}} \right), \quad (247b)$$

$$I_3 = \int_{2M}^r dr' \Phi_{\text{bot}}^{-1} \left(\delta \hat{A} \hat{\psi}_-^{\text{ret}} + \hat{\mathcal{D}} \hat{\varphi}_H^{\mathcal{P}} \right), \quad (247c)$$

$$I_4 = \int_r^{\infty} dr' \Phi_{\text{top}}^{-1} \left(\delta \hat{A} \hat{\psi}_+^{\text{ret}} + \hat{\mathcal{D}} \hat{\varphi}_{\infty}^{\mathcal{P}} \right), \quad (247d)$$

$$I_5 = \int_{2M}^{r_0} dr' \Phi_{\text{bot}}^{-1} \left(\delta \hat{A} \hat{\psi}_-^{\text{ret}} + \hat{\mathcal{D}} \hat{\varphi}_H^{\mathcal{P}} \right), \quad (247e)$$

$$I_6 = \int_{r_0}^r dr' \Phi_{\text{bot}}^{-1} \left(\delta \hat{A} \hat{\psi}_+^{\text{ret}} + \hat{\mathcal{D}} \hat{\varphi}_{\infty}^{\mathcal{P}} \right). \quad (247f)$$

In t slicing, $\delta \hat{A}$ reduces to

$$\delta \hat{A}_{[t]} = 2\omega \delta\omega \begin{pmatrix} \mathbf{0}_{d \times d} & \mathbf{0}_{d \times d} \\ \mathbf{1}_{d \times d} & \mathbf{0}_{d \times d} \end{pmatrix}. \quad (248)$$

Given Eq. (245), the contribution \mathbf{v}_2 simplifies more significantly. After some manipulations involving integration by parts, we find

$$\mathbf{v}_2 = \mathbf{v}_2^- \theta(r_0 - r) + \mathbf{v}_2^+ \theta(r - r_0) - \Phi_0^{-1} \hat{J}^{\text{PP}} \delta(r - r_0), \quad (249)$$

with

$$\mathbf{v}_2^- = \begin{pmatrix} -\Phi_{0,\text{top}}^{-1} \left[\delta \hat{J}^{\text{PP}} + \hat{A}_0 \hat{J}^{\text{PP}} \right] \\ \mathbf{0}_d \end{pmatrix}, \quad (250a)$$

$$\mathbf{v}_2^+ = \begin{pmatrix} \mathbf{0}_d \\ \Phi_{0,\text{bot}}^{-1} \left[\delta \hat{J}^{\text{PP}} + \hat{A}_0 \hat{J}^{\text{PP}} \right] \end{pmatrix}. \quad (250b)$$

Here the factor $\hat{A}_0 := \hat{A}(r_0)$ has appeared after applying the identity (139).

3. $\partial_{r_0} \bar{h}_{i\ell m}^{(1)}$ on v - t - u slices

We obtain $\partial_{r_0} \bar{h}_{[vtu]}^{(1)}$ using Eq. (197). With this slicing, no punctures are required.

In $\mathbf{v}_{\varphi} = \mathbf{v}_1 + \mathbf{v}_2$, \mathbf{v}_1 is again given by Eq. (246), but now with $\hat{\varphi}_a^{\mathcal{P}} = 0$. $\delta \hat{A}$ is now given by

$$\delta \hat{A}_{[v]} = \begin{pmatrix} \mathbf{0}_{d \times d} & \mathbf{0}_{d \times d} \\ \delta \mathcal{M}_h & -2imf^{-1} \delta \Omega \mathbf{1}_{d \times d} \end{pmatrix} \text{ for } r \in \Gamma_H, \quad (251)$$

$$\delta \hat{A}_{[u]} = \begin{pmatrix} \mathbf{0}_{d \times d} & \mathbf{0}_{d \times d} \\ \delta \mathcal{M}_h & 2imf^{-1} \delta \Omega \mathbf{1}_{d \times d} \end{pmatrix} \text{ for } r \in \Gamma_{\infty}, \quad (252)$$

and by Eq. (248) for $r \in \Gamma_p$. $\delta \mathcal{M}_h$ is given explicitly in Eqs. (A15) and (A16), with $H = -1$ in $\delta \hat{A}_{[v]}$ and $H = +1$ in $\delta \hat{A}_{[u]}$.

The contribution \mathbf{v}_2 is given by Eq. (249), unchanged from t slicing.

4. Results and comparison between slicings

Figures 4 and 5 show our results for the $\ell = 2, m = 2$ mode of $\partial_{r_0} \bar{h}_{[t]}^{(1)}$ and $\partial_{r_0} \bar{h}_{[vtu]}^{(1)}$. These fields are generically discontinuous at $r = r_0$ due to the $\delta'(r - r_0)$ source. $\partial_{r_0} \bar{h}_{[vtu]}^{(1)}$ additionally contains discontinuities at the boundaries between slicings, as $\bar{h}_{[vtu]}^{(1)}$ did. At large r , $\partial_{r_0} \bar{h}_{[t]}^{(1)}$ oscillates with growing amplitude, while $\partial_{r_0} \bar{h}_{[vtu]}^{(1)}$ goes to a constant. This is reinforced in Fig. 6, which shows the absolute value $|\partial_{r_0} \bar{h}_{[t]}^{(1)}|$ growing at large r while $|\partial_{r_0} \bar{h}_{[vtu]}^{(1)}|$ decays to a constant. Similar differences in behavior would appear near the horizon if the plots were to zoom in on that region.

To compare our results in the two slicings, we transform from t to v - t - u slicing using

$$\begin{aligned} \delta \bar{h}_{[vtu]}^{(1)} &= \delta \left(e^{-i\omega_m k(r^*)} \bar{h}_{[t]}^{(1)} \right) \\ &= e^{-i\omega_m k(r^*)} \left(\delta \bar{h}_{[t]}^{(1)} - i\delta\omega_m k(r^*) \bar{h}_{[t]}^{(1)} \right). \end{aligned} \quad (253)$$

We find a relative difference $\lesssim 10^{-11}$ after performing this transformation, confirming the consistency of our results for different slicings.

X. DEMONSTRATION 2: TEUKOLSKY CALCULATIONS FOR QUASICIRCULAR ORBITS

In this section we apply our scheme to the calculation of the first-order $s = -2$ Teukolsky master function and its derivative with respect to an orbital parameter. This problem is slightly different in structure than the Lorenz-gauge problem explored in Sec. IX, but the generic method is still applicable. The equations we solve still have the forms of Eqs. (230) and (240), simply with different differential operators and source terms.

A. Calculation of ${}_{-2}R_{\ell m}$

As in the Lorenz-gauge case, we first review the calculation of the first-order retarded solution.

For a particle on a quasicircular orbit of (leading-order) radius r_0 , the Teukolsky master function for the first-order perturbed Weyl scalar, $\psi_4^{(1)} = \psi_4[h^{(1)}]$, is given by Eq. (230) with $\hat{\psi}^{(1)} = ({}_{-2}R_{\ell m}, \partial_r ({}_{-2}R_{\ell m}))^T$ and with $\hat{\mathcal{D}}$ now defined by the matrices A and B given in Eq. (106).

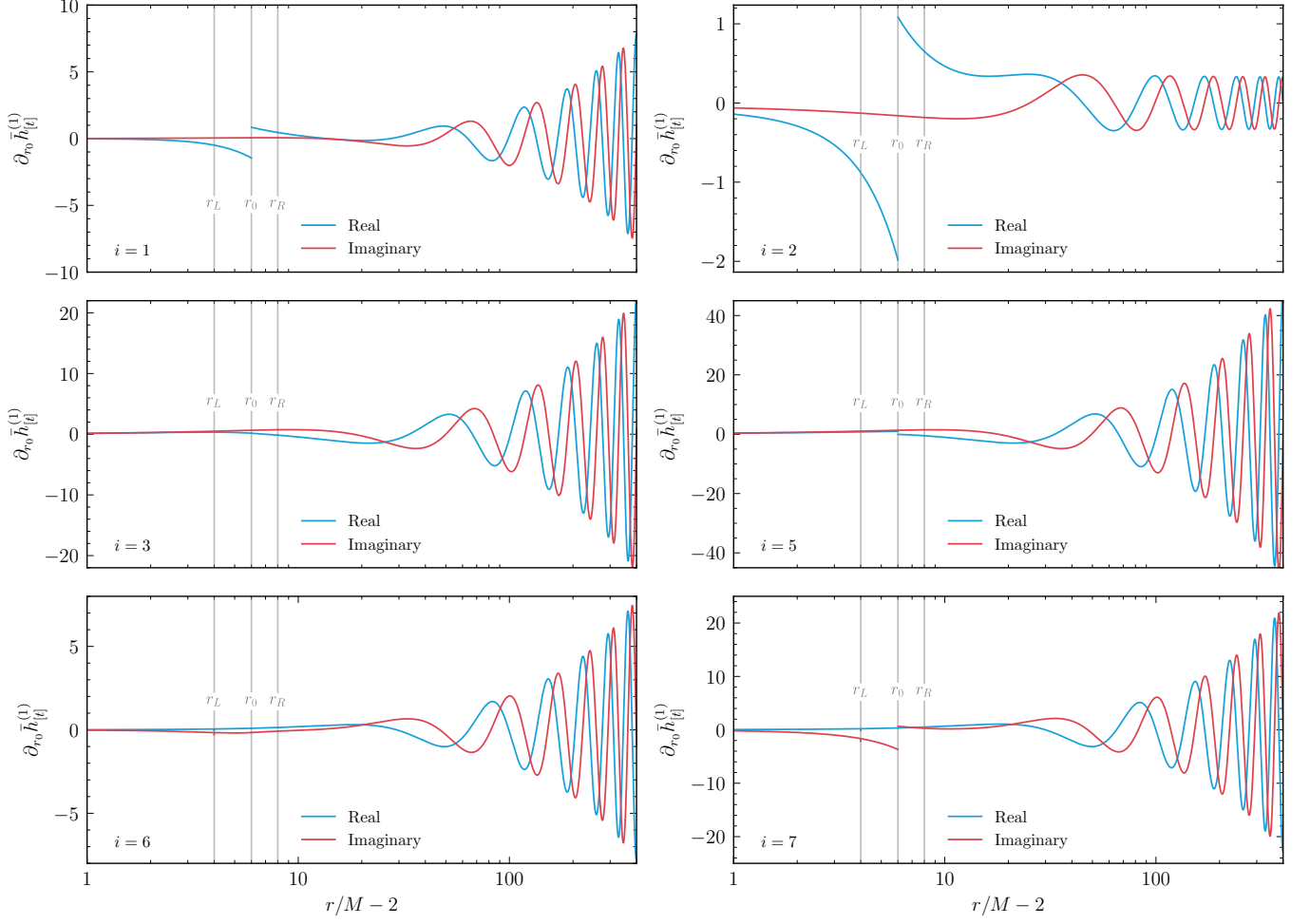


FIG. 4. Real and imaginary parts of $\partial_{r_0} \bar{h}_{[\ell]}^{(i)}$ for all nonvanishing i modes with $\ell = 2$, $m = 2$, $r_0 = 8M$. Note that we have not included the $i = 4$ BLS mode in this figure for brevity as this is qualitatively the same as the $i = 1$ mode.

The point-particle source for the Teukolsky master function has further distributional content than the Lorenz-gauge source in Eq. (231), such that

$$\hat{J}^{(1)} = \hat{J}_{\text{pp}}^{(A)}(r_0)\delta(r - r_0) + \hat{J}_{\text{pp}}^{(B)}(r_0)\delta'(r - r_0) + \hat{J}_{\text{pp}}^{(C)}(r_0)\delta''(r - r_0), \quad (254)$$

where $\hat{J}_{\text{pp}}^{(i)} = (0, J_{\text{pp}}^{(i)})^T$ with $i \in \{A, B, C\}$. $J_{\text{pp}}^{(i)}$ are the source terms given in Appendix C.

The retarded point-particle solution for the Teukolsky master function is given by Eq. (124). But the additional distributional content in the source leads to \mathbf{v} having a similar schematic form to Eq. (249) for $\partial_{r_0} \bar{h}_{i\ell m}^{(1)}$, as opposed to Eq. (235) for $\bar{h}_{i\ell m}^{(1)}$. We write this as $\mathbf{v} = \mathbf{v}_\theta + \mathbf{v}_\delta$, where

$$\mathbf{v}_\theta = \mathbf{v}_\theta^- \theta(r_0 - r) + \mathbf{v}_\theta^+ \theta(r - r_0), \quad (255)$$

$$\mathbf{v}_\delta = \Phi_0^{-1} [\mathbf{1}\delta'(r - r_0) - \mathbf{R}\delta(r - r_0)] \hat{J}_{\text{pp}}^{(C)}. \quad (256)$$

Here $\mathbf{R} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ is a reflection matrix such that

$\mathbf{R} \hat{J}_{\text{pp}}^{(C)} = (J_{\text{pp}}^{(C)}, 0)^T$. The quantities \mathbf{v}_θ^- and \mathbf{v}_θ^+ are found through integration by parts, which yields

$$\mathbf{v}_\theta^- = \begin{pmatrix} -\Phi_{0,\text{top}}^{-1} \left[\hat{J}_{\text{pp}}^{(A)} - \hat{A}_0 \hat{J}_{\text{pp}}^{(B)} + (\hat{A}_0^2 + \partial_r \hat{A}_0) \hat{J}_{\text{pp}}^{(C)} \right] \\ 0 \end{pmatrix}, \quad (257)$$

$$\mathbf{v}_\theta^+ = \begin{pmatrix} 0 \\ \Phi_{0,\text{bot}}^{-1} \left[\hat{J}_{\text{pp}}^{(A)} - \hat{A}_0 \hat{J}_{\text{pp}}^{(B)} + (\hat{A}_0^2 + \partial_r \hat{A}_0) \hat{J}_{\text{pp}}^{(C)} \right] \end{pmatrix}, \quad (258)$$

where we have used the relation in Eq. (139) and its derivative: $\frac{d^2 \Phi^{-1}}{dr^2} = \Phi^{-1} \left(\hat{A}^2 + \frac{d\hat{A}}{dr} \right)$.

The solution is evaluated in the following manner:

1. Fix a zeroth-order orbital radius r_0 .
2. For each ℓm mode, we construct a matrix of homogeneous solutions, Φ , as explained in Appendix B 2.
3. Calculate the retarded field for the column vector $\hat{\psi}^{(1)}$ using Eq. (124) with $\mathbf{v} = \mathbf{v}_\theta + \mathbf{v}_\delta$ given by

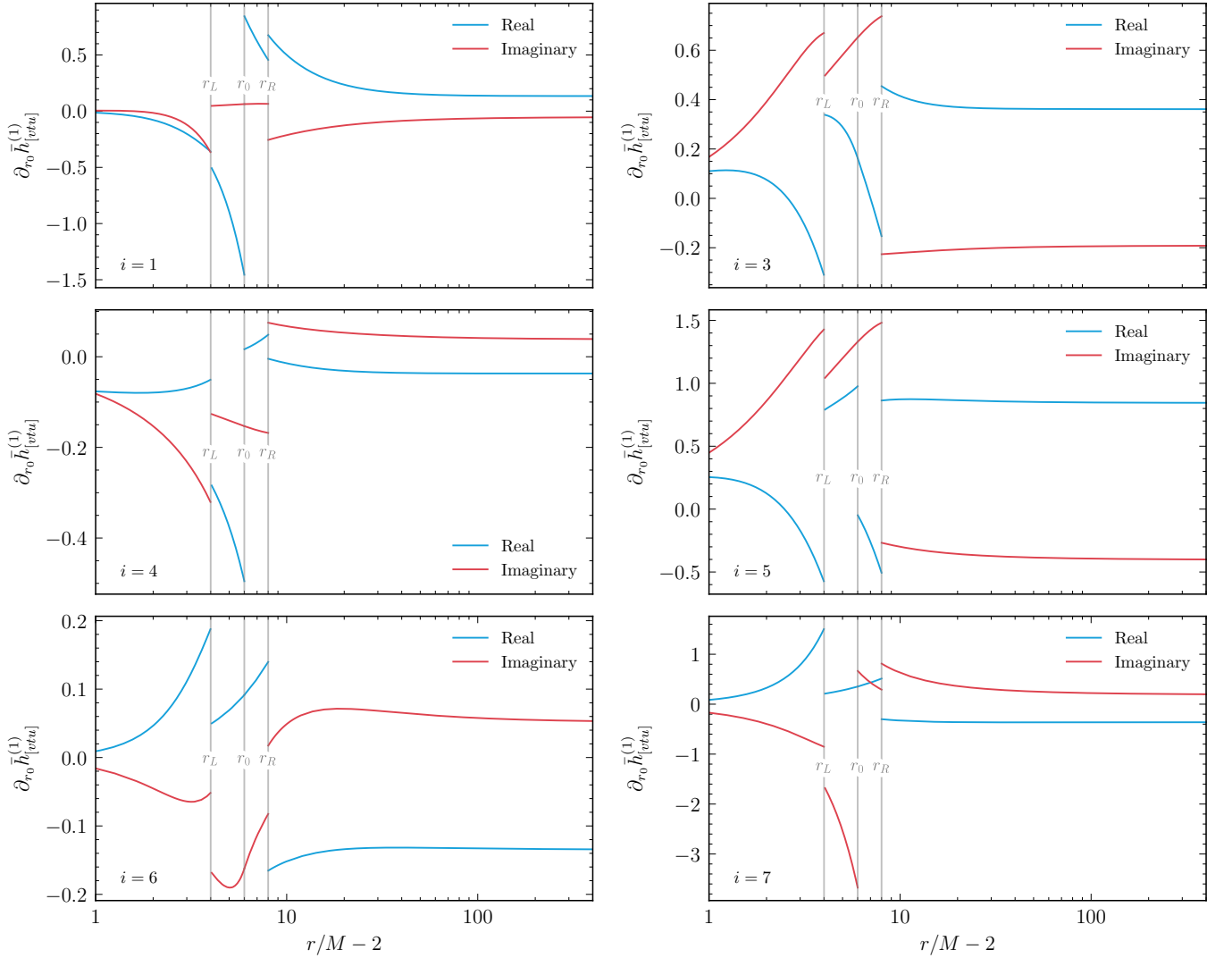


FIG. 5. Real and imaginary parts of $\partial_{r_0} \bar{h}_{[vtu]}^{(1)}$ for all nonvanishing i modes with $\ell = 2, m = 2, r_0 = 8M$. Note that we have not included the $i = 2$ BLS mode in this figure for brevity as this is qualitatively the same as the $i = 1$ mode.

Eqs. (255)-(256). The inversion of the matrix Φ for the calculation of \mathbf{v} is facilitated by *Mathematica's* **Inverse** routine.

- Although written in a different manner, this solution is entirely equivalent to the solutions in the literature [4, 61–64] and can be readily computed using the Teukolsky package in the Black Hole Perturbation Toolkit (BHPTToolkit) [65]. This provides a robust check of our numerical results for the retarded field and we find relative differences of $\lesssim 10^{-12}$ between our calculation and the BHP-Toolkit.

B. Calculation of $\partial_{r_0} (-_2R_{\ell m})$

1. Overview

After reviewing the retarded point-particle solution, we now move on to the calculation of its derivative with respect to an orbital parameter. Like in the Lorenz-gauge case, the field equation we consider is Eq. (240), but now with $\varphi^{\text{ret}} = \delta \hat{\psi}^{(1)} = (\delta -_2R_{\ell m}, \partial_r (\delta -_2R_{\ell m}))^T$. The source term, $K^{(1)}$, has the same form as Eq. (241), but the first, extended term has added distributional content,

$$\begin{aligned} \delta \hat{A} \hat{\psi}^{(1)} &= \delta \hat{A} \hat{\psi}_-^{(1)} \theta(r_0 - r) + \delta \hat{A} \hat{\psi}_+^{(1)} \theta(r - r_0) \\ &\quad - \delta \hat{A} \hat{J}_{\text{pp}}^{(C)} \delta(r - r_0). \end{aligned} \quad (259)$$

The extended support from the source term again originates from the retarded point particle (Teukolsky) solu-

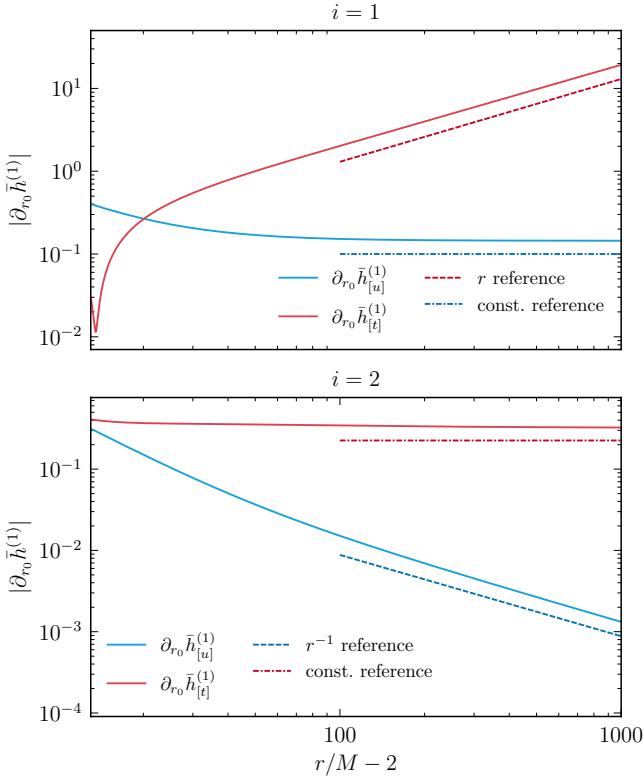


FIG. 6. Comparison between $|\partial_{r_0} \bar{h}_{[u]}^{(1)}|$ (blue line) and $|\partial_{r_0} \bar{h}_{[t]}^{(1)}|$ (red line) for $i = 1$ (top panel) and $i = 2$ (bottom panel) with $\ell = 2, m = 2, r_0 = 8M$.

tion, $\hat{\psi}_{\pm}^{(1)} = \Phi v_{\pm}$. Explicitly, δA and δB for the Teukolsky problem have the following form:

$$\delta A = 2f^{-2} \left[(1 - H^2) \omega_m \delta \omega_m - 2\omega_m^2 H \delta H - \delta_{-2} V_{\ell m}(r) \right], \quad (260a)$$

$$\delta B = 2if^{-1} (\delta \omega_m H + \omega_m \delta H), \quad (260b)$$

where

$$\delta_{-2} V_{\ell m}(r) = 4ir^{-2} \{ \delta \omega_m [r(1 - H)f - M(1 + H)] - rf \delta H - M \delta H \}. \quad (261)$$

The secondary source term arising from the derivative of the point-particle Teukolsky source is written concisely as

$$\begin{aligned} \delta \hat{J}^{(1)} = & \left[\delta \hat{J}_{\text{pp}}^{(A)} \delta(r - r_0) + \delta \hat{J}_{\text{pp}}^{(B)} \delta'(r - r_0) \right. \\ & + \delta \hat{J}_{\text{pp}}^{(C)} \delta''(r - r_0) - \hat{J}_{\text{pp}}^{(A)} \delta'(r - r_0) \\ & \left. - \hat{J}_{\text{pp}}^{(B)} \delta''(r - r_0) - \hat{J}_{\text{pp}}^{(C)} \delta'''(r - r_0) \right]. \quad (262) \end{aligned}$$

The solution is given by Eq. (202). Due to the more complicated source, the quantity v_{φ} , defined in Eq. (175),

has a more complicated form than in the Lorenz gauge:

$$\begin{aligned} v_{\varphi} = & v_3 + v_4 + v_5 + v_6 \\ & + \Phi_0^{-1} [\mathbf{R} \delta(r - r_0) + \mathbf{1} \delta'(r - r_0)] \left(\hat{J}_{\text{pp}}^{(B)} - \delta \hat{J}_{\text{pp}}^{(C)} \right) \\ & + \Phi_0^{-1} [\mathbf{R} \delta'(r - r_0) + \mathbf{1} \delta''(r - r_0)] \hat{J}_{\text{pp}}^{(C)}. \quad (263) \end{aligned}$$

The terms v_3 and v_6 originate from the source $\delta \hat{A} \hat{\psi}^{(1)}$ [i.e., they comprise v_1 in Eq. (175)], while all other terms originate from the source $\delta \hat{J}^{(1)}$ [i.e., they comprise v_2 in Eq. (175)].

v_3 specifically corresponds to the integral over the Heaviside terms in Eq. (259), meaning it has the form given in Eq. (246) and accounts for the integration over the extended piece of the source. v_6 is then the integral over the delta term in Eq. (259):

$$v_6 = v_6^- \theta(r_0 - r) + v_6^+ \theta(r - r_0). \quad (264)$$

Here v_6^{\pm} are given concisely by

$$v_6^- = \begin{pmatrix} -\Phi_{0,\text{top}}^{-1} \delta \hat{A}_0 \hat{J}_{\text{pp}}^{(C)} \\ 0 \end{pmatrix}, \quad v_6^+ = \begin{pmatrix} 0 \\ \Phi_{0,\text{bot}}^{-1} \delta \hat{A}_0 \hat{J}_{\text{pp}}^{(C)} \end{pmatrix}. \quad (265)$$

The rest of the terms follow immediately from the general formula (177) for v_2 with $\delta \hat{J}$ given by Eq. (262). v_4 represents the integral of the first set of delta functions in Eq. (262), from which one finds

$$v_4 = v_4^- \theta(r_0 - r) + v_4^+ \theta(r - r_0), \quad (266)$$

where

$$v_4^- = \begin{pmatrix} -\Phi_{0,\text{top}}^{-1} \left[\delta \hat{J}_{\text{pp}}^{(A)} - \hat{A}_0 \delta \hat{J}_{\text{pp}}^{(B)} + (\hat{A}_0^2 + \partial_r \hat{A}_0) \delta \hat{J}_{\text{pp}}^{(C)} \right] \\ 0 \end{pmatrix}, \quad (267)$$

$$v_4^+ = \begin{pmatrix} 0, \\ \Phi_{0,\text{bot}}^{-1} \left[\delta \hat{J}_{\text{pp}}^{(A)} - \hat{A}_0 \delta \hat{J}_{\text{pp}}^{(B)} + (\hat{A}_0^2 + \partial_r \hat{A}_0) \delta \hat{J}_{\text{pp}}^{(C)} \right] \end{pmatrix}. \quad (268)$$

The next term, v_5 , arises from the second grouping of delta functions in Eq. (262) and hence follows the same split as Eq. (266),

$$v_5 = v_5^- \theta(r_0 - r) + v_5^+ \theta(r - r_0). \quad (269)$$

However, the higher-order derivatives of the delta functions than seen previously requires one higher derivative of Eq. (139), leading to

$$\frac{d^3 \Phi^{-1}}{dr^3} = \Phi^{-1} \left(\hat{A} \frac{d\hat{A}}{dr} + \frac{d\hat{A}}{dr} \hat{A} + \hat{A}^3 + \hat{A} \frac{d\hat{A}}{dr} + \frac{d^2 \hat{A}}{dr^2} \right). \quad (270)$$

Using this relation one finds

$$\mathbf{v}_5^- = \begin{pmatrix} \Phi_{0,\text{top}}^{-1} \left[\hat{A}_0 \hat{J}_{\text{pp}}^{(A)} - (\hat{A}_0^2 + \partial_r \hat{A}_0) \hat{J}_{\text{pp}}^{(B)} + (\hat{A}_0 \partial_r \hat{A}_0) \right. \\ \left. + \partial_r \hat{A}_0 \hat{A}_0 + \hat{A}_0^3 + \hat{A}_0 \partial_r \hat{A}_0 + \partial_r^2 \hat{A}_0 \right] \hat{J}_{\text{pp}}^{(C)} \\ 0 \end{pmatrix}, \quad (271)$$

$$\mathbf{v}_5^+ = \begin{pmatrix} 0 \\ -\Phi_{0,\text{bot}}^{-1} \left[\hat{A}_0 \hat{J}_{\text{pp}}^{(A)} - (\hat{A}_0^2 + \partial_r \hat{A}_0) \hat{J}_{\text{pp}}^{(B)} + (\hat{A}_0 \partial_r \hat{A}_0) \right. \\ \left. + \partial_r \hat{A}_0 \hat{A}_0 + \hat{A}_0^3 + \hat{A}_0 \partial_r \hat{A}_0 + \partial_r^2 \hat{A}_0 \right] \hat{J}_{\text{pp}}^{(C)} \end{pmatrix}. \quad (272)$$

2. $\partial_{r_0} R_{[vtu]}$ on v - t - u slices

Our calculation of $\partial_{r_0} R_{[vtu]}$ is done through Eq. (202), with \mathbf{v}_φ given by Eq. (263), but within the integrals of the source terms in \mathbf{v}_3 , we include no puncture in the regions where $r \in \Gamma_p$ as we are only considering the retarded solution. Furthermore, we choose not to include a puncture toward the horizon, where $r \in \Gamma_H$, as we find Eq. (147) is satisfied for a fiducial horizon puncture. Hence in the integrals I_i that enter \mathbf{v}_3 , with $i \in \{1, \dots, 6\}$, we set $\hat{\varphi}_H^P = \hat{\varphi}_p^P = 0$.

In the Teukolsky framework (with $s = -2$), $\delta \hat{A}$ is now given in the various slicings by

$$\delta \hat{A}_{[v]} = 2m f^{-1} \delta \Omega \begin{pmatrix} 0 & 0 \\ 4r^{-1} & 1 \end{pmatrix}, r \in \Gamma_H, \quad (273)$$

$$\delta \hat{A}_{[t]} = 2m f^{-2} \delta \omega_m \begin{pmatrix} 0 & 0 \\ 2r^{-2}(rf - M) + i\omega_m & 0 \end{pmatrix}, r \in \Gamma_p, \quad (274)$$

$$\delta \hat{A}_{[u]} = -2m f^{-1} \delta \Omega \begin{pmatrix} 0 & 0 \\ 4r^{-2} & 1 \end{pmatrix}, r \in \Gamma_\infty. \quad (275)$$

$\delta \hat{A}$, shown in Fig. 7, forms a central component of the overall source term. We see that this piece diverges as $\sim f^{-1}$ toward the horizon but converges toward infinity. However, to determine whether the retarded integrals converge, we must analyse the entire integrands.

Figure 8 plots the integrands in Eq. (247), both with and without punctures. As shown by the reference curves in the two plots, the integrands $\Phi_{\text{top}}^{-1} \delta \hat{A} \hat{\psi}_-^{\text{ret}}$ and $\Phi_{\text{bot}}^{-1} \delta \hat{A} \hat{\psi}_+^{\text{ret}}$ converge toward the horizon as $\sim f^2$ and $\sim f^0$, respectively. The analogous integrands, however, diverge as $\sim r^2$ toward null infinity, verifying the need for a puncture in the region Γ_∞ .

Construction of appropriate punctures in this context was discussed in Sec. VIID 2. We show the application of these punctures in improving the falloff of the integrands in the region Γ_∞ in Fig. 8. Here we used the asymptotic expansion in Eq. (206) with $j_{\text{max}} = 4$. The plot shows how the inclusion of the puncture now forces the integrands to fall off as $\sim r^{-3}$ and therefore leave us with a finite integral. Punctures could be constructed in a

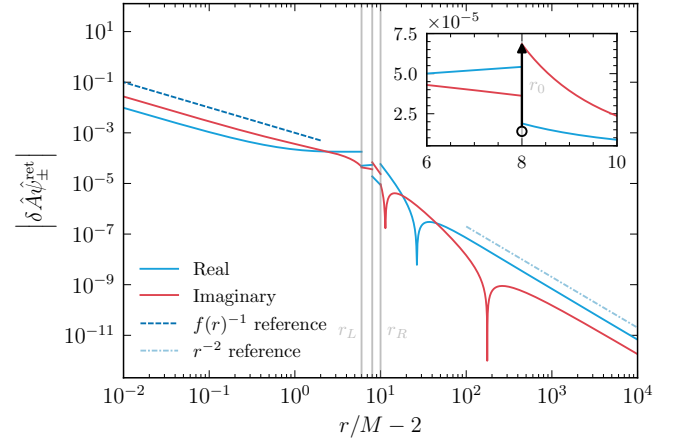


FIG. 7. Real and imaginary parts of the extended source terms appearing in the integrands within Eq. (246) for \mathbf{v}_3 . In the asymptotic regions, the source decays as $\sim r^{-2}$ toward spatial infinity but grows as $\sim f^{-1}$ toward the horizon. Here $\ell = 2$, $m = 2$ and the secondary is at $r_0 = 10M$. The vertical arrow in the inset of the plot signifies the presence of additional distributional pieces that must be taken into account when calculating the full solution.

similar manner in the other asymptotic region, Γ_H . This would speed up the convergence of the integration over this region, but it is not required.

In Fig. 9, we present results for the $\ell = 2$, $m = 2$ mode of $\partial_{r_0} (-2R_{[vtu]})$. As is evident from the form of the solution in Eq. (263), the solution is discontinuous at the particle's location, owing to the Dirac delta primes that appear in the source. Furthermore, there are also jumps at the boundaries of the regions r_L and r_R due to the change in slicing there.

3. $\partial_{r_0} R_{[t]}$ on t slices

For comparison purposes we also present in Fig. 10 the same results after transforming to t slicing throughout the numerical domain. As we observed in Fig. 3, we see that $\partial_{r_0} (-2R_{[t]})$ contains constant-amplitude oscillations at large r that are not present in the solution for $\partial_{r_0} (-2R_{[vtu]})$. Also, in t slicing, there will be oscillations toward the horizon, but the aspect ratio and choice of radial coordinate preclude them from being seen in Fig. 3.

XI. CONCLUSION AND OUTLOOK

In this paper we have formulated a worldtube puncture scheme for self-force calculations in the Fourier domain. We have specifically focused on the types of field equations that arise in a multiscale expansion of the Einstein equation, but the method applies equally well in an ordinary frequency-domain calculation.

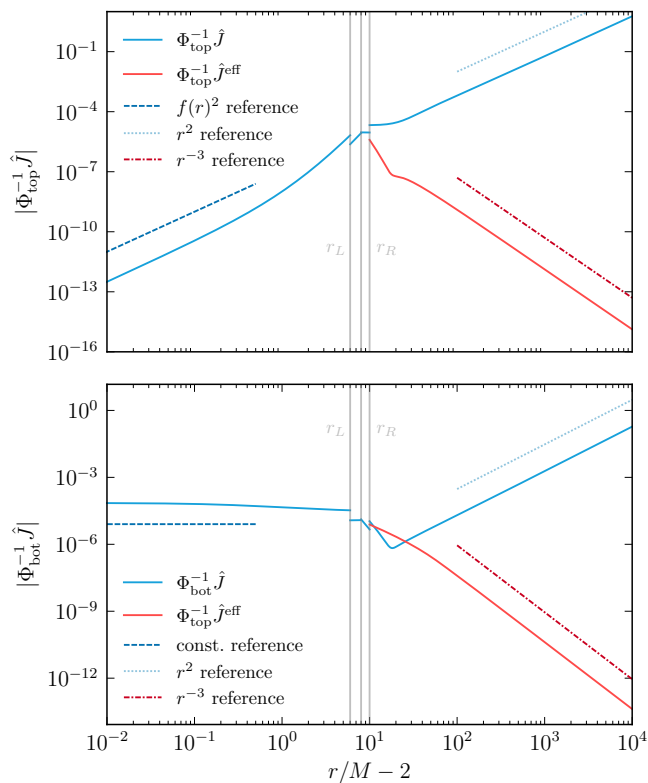


FIG. 8. Comparison of the non-punctured and punctured integrands for the extended source terms within the integrals appearing in Eq. (246) for v_3 . *Top panel:* The integrands of the weighting coefficient for the homogeneous solutions Φ_- throughout the entire numerical domain. In the absence of a puncture, the integrand falls off as $\sim f^2$ toward the horizon but grows as $\sim r^2$ toward null infinity. Therefore in the region Γ_∞ we apply a suitable puncture to make the integral converge. The puncture used in the figure ensures the integrand now falls off as $\sim r^{-3}$ toward null infinity. *Bottom panel:* The integrands of the weighting coefficient for the homogeneous solutions Φ_+ throughout the entire numerical domain. Without a puncture (blue curve), the integrand tends to a constant toward the horizon but again grows as $\sim r^2$ toward null infinity. With the puncture (red curve) applied in Γ_∞ , the integrand again falls off as $\sim r^{-3}$.

We have also demonstrated our scheme’s utility and flexibility by numerically implementing it both for the Lorenz-gauge field equations and the Teukolsky equation. Moreover, we note that although it is described here for the first time, our method has already been successfully employed more broadly; it underlay all second-order calculations to date [7, 17, 18].

However, in the time since our method was first formulated and implemented, at least two alternatives have been presented that offer some clear advantages [29, 36]. It is therefore worth making a careful assessment of the relative merits of these various approaches. It is also important to point out some aspects of our method that can be usefully carried over to those other schemes (and vice versa).

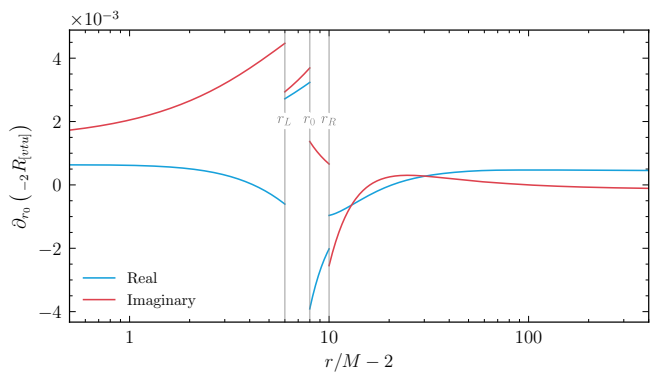


FIG. 9. Real and imaginary parts of $\partial_{r_0} (-_2 R_{[vtu]})$ with $\ell = 2$, $m = 2$, $r_0 = 10M$.

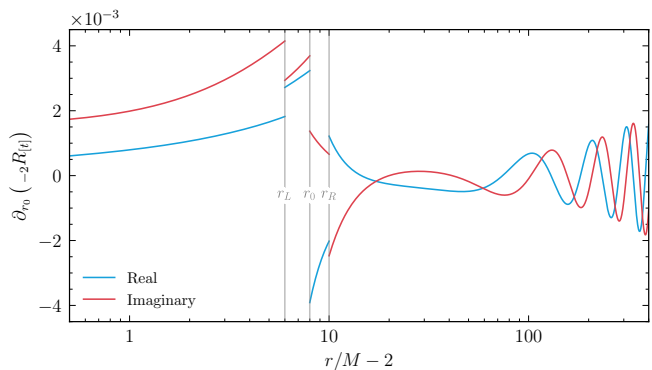


FIG. 10. Real and imaginary parts of $\partial_{r_0} (-_2 R_{[t]})$ with $\ell = 2$, $m = 2$, $r_0 = 10M$.

We first observe that our scheme is substantially more general than earlier worldtube puncture schemes. It is intrinsically a multi-domain method, and it exploits that flexibility by (i) accommodating punctures in multiple domains and (ii) allowing different choices of time slicing (and therefore different field equations) in different domains. This type of generality could be beneficial in any approach.

In terms of practical implementation, the key difference between our scheme and the alternatives is that we apply the method of variation of parameters for sources with spatially unbounded support. This approach obtains inhomogeneous solutions by convolving homogeneous solutions against the source, a procedure with substantial drawbacks when the source has unbounded support. One drawback is that the homogeneous solutions need to be known at all radii. This is problematic because the ‘up’ solutions (i.e., the homogeneous solutions that are regular at \mathcal{S}^+) need to be calculated near the horizon, and similarly the ‘in’ solutions (i.e., the homogeneous solutions that are regular at \mathcal{H}^+) need to be calculated at large radius. It can be difficult to accurately compute these homogeneous solutions far away from where their numerical boundary conditions are specified. A second drawback is that the method sacri-

fices some of the advantages of hyperboloidal slicing. On these slices, the retarded inhomogeneous solution varies slowly across the domain, with no oscillations at large r or near the horizon; this means, in principle, no oscillations need to be numerically resolved. The ‘up’ solutions share this property at large r , and the ‘in’ solutions share it near the horizon. However, each of these homogeneous solutions oscillates in the opposite domain: ‘up’, near the horizon; and ‘in’, at large r . This means that to evaluate the variation-of-parameters integrals, we must resolve the oscillations even though we are guaranteed that they do not appear in the ultimate, retarded solution.

These two drawbacks can be tempered by the use of higher-order punctures in the horizon and infinity regions to force the source to fall off more rapidly and thus reduce the contributions from the undesirable homogeneous solutions in each region. We do take that approach in Refs. [7, 17, 18]. But the alternative approaches in Refs. [29, 36] have more elegantly circumvented the issues that arise in variation of parameters.

The first alternative approach uses the method of partial annihilators [66]. This method can be applied when there exists an operator which when applied to the source takes it from unbounded support to pointlike (i.e., measure-zero) support. Acting with this operator on the whole field equation results in a higher-order differential equation with a distributional source. This new equation can then be solved with variation of parameters, and each homogeneous solution is only required in the region where it is well behaved. Such a partial annihilator operator exists for the calculation of parametric derivatives, and this approach has been employed for the r_0 derivatives of the Regge-Wheeler-Zerilli master variables and Lorenz-gauge perturbations [36]. A limitation in this approach is that it is unlikely that a partial annihilator operator exists for the full second-order calculation.

The second alternative approach leaves the source intact but directly solves the field equation in each domain using a spectral method rather than through convolution with homogeneous solutions. Like our scheme, this approach is naturally suited to multi-domain techniques. Because it does not involve a basis of homogeneous solutions, it is better adapted to hyperboloidal slicing: rather than having to resolve oscillatory homogeneous solutions near \mathcal{H}^+ and \mathcal{I}^+ , one only deals with slowly varying functions, allowing one to compactify the numerical domain; and rather than having to construct high-order asymptotic expansions to impose boundary conditions on the homogeneous solutions, the field equation itself imposes boundary conditions on the retarded solution at \mathcal{H}^+ and \mathcal{I}^+ . We expand on the latter point below. This multi-domain, spectral, compactified hyperboloidal approach was implemented for a scalar-field toy-model in Ref. [29]. In that work the method was shown to be very efficient for distributional sources, extended sources, and sources with unbounded support, where for the latter the calculation of a parametric r_0 derivative was used as an example.

Despite variation of parameters’ disadvantages, it does have some clear advantages. One benefit is that it is a straightforward way of solving problems with complicated distributional sources. For example, in Ref. [37], the source for the second-order retarded metric perturbation was shown to have the form of a highly nontrivial limit of a sequence of distributions. Dealing with such sources is simplest if one can write the solution immediately as an integral against a Green’s function, as in variation of parameters, and then manipulate the integral (e.g., through integration by parts) before any numerical evaluation. Hence, a valuable approach might be to combine methods, using variation of parameters within a domain containing the particle and alternative methods outside that domain.

We also wish to stress that most obstacles encountered in our complete second-order calculations are independent of our use of variation of parameters. As mentioned above, one advantage of compactified hyperboloidal slicing is that it can avoid the need to calculate boundary conditions. More precisely, if the numerical variable is regular at the compactified boundaries, then the field equations themselves reduce to regularity conditions at the boundaries, and there is no need to construct boundary conditions of the form described in Appendix B. However, this does not mean boundary conditions never need to be calculated, nor does it mean that punctures are unnecessary. At second order, we do not generically have regular fields at the boundaries: as analyzed in Ref. [33] and alluded to in Sec. III D, the second-order solution in the multiscale expansion is irregular at the boundaries. The correct physical boundary conditions for the multiscale field equations can be derived from a post-Minkowski expansion near \mathcal{I}^+ and an analogous expansion near the horizon. These physical boundary conditions contain hereditary terms, integrals over the system’s entire past history, which are impossible to determine from the field equations in the numerical domain, regardless of one’s choice of slicing or compactification.

The framework in this paper readily incorporates such boundary conditions into punctures at the boundaries. Our analysis in Sec. V C also provides a diagnostic for when a puncture is required and the conditions it must satisfy. That type of analysis should continue to serve a key purpose even when the method of variation of parameters is not used.

We also note that other aspects of our scheme are independent of the use of variation of parameters. One obvious example is the overarching multiscale method, which we have presented in a more geometrical way than in previous literature. Derivatives of the numerical fields with respect to orbital parameters are an essential ingredient in that method [2] and in closely associated ones [67–69]. Our analysis has highlighted how calculations of such parametric derivatives depend crucially on the choice of slicing. If standard, constant- t slicing is used, infrared divergences arise. Such divergences can be treated by introducing punctures at the horizon and in-

finitly to enforce physical boundary conditions. However, hyperboloidal slicing entirely evades these divergences (at least for broad classes of fields).

Followup papers will explain how the second-order self-force results in Refs. [7, 17, 18] were obtained by combining (i) the puncture scheme in this paper, (ii) the punctures in Ref. [38], (iii) the coupling formulas presented in Ref. [34], (iv) the multiscale expansion of the Lorenz-gauge field equations in Ref. [9] (reviewed in this paper), and (v) the strategies developed in Refs. [33, 70] to overcome infrared divergences and poor convergence of mode sums.

In the longer term, our scheme can be applied to eccentric orbits [71]. As we emphasised throughout the body of this paper, the bulk of our analysis applies equally well for eccentric as for quasicircular orbits.

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Appendix A: Coupling matrices and operators in the Lorenz-gauge field equations

In this appendix we give explicit expressions for the quantities $\mathcal{M}_{ij}^{(n)}$, \mathcal{M}_h , $\mathcal{M}_{\partial h}$, $\delta\mathcal{M}_h$, and $Z_{kj}^{(n)}$ appearing in the Lorenz-gauge equations (59) [via (60) and (65)]; (69) [via (73)]; (168) [via (244)]; and the gauge conditions (67) and (68). For brevity, we omit ℓm labels on the fields \bar{h}_{ilm} and frequency ω_m , and we follow Ref. [9] by adopting the shorthand

$$\lambda := (\ell + 2)(\ell - 1) \quad \text{and} \quad \lambda_1 := \ell(\ell + 1). \quad (\text{A1})$$

1. Coupling matrices

The quantities $\mathcal{M}_{ij}^{(0)} \bar{h}_j$ in Eq. (60) are given by

$$\mathcal{M}_{1j}^{(0)} \bar{h}_j = \frac{f^2 f'}{2} \left(\partial_r \bar{h}_3 + \frac{i\omega H}{f} \bar{h}_3 \right) + \frac{f \left(1 - \frac{4M}{r} \right)}{2r^2} (\bar{h}_1 - \bar{h}_5 - f \bar{h}_3) - \frac{f^2}{2r^2} \left(1 - \frac{6M}{r} \right) \bar{h}_6, \quad (\text{A2})$$

$$\begin{aligned} \mathcal{M}_{2j}^{(0)} \bar{h}_j &= \frac{f^2 f'}{2} \left(\partial_r \bar{h}_3 + \frac{i\omega H}{f} \bar{h}_3 \right) + \frac{f f'}{2} \partial_r (\bar{h}_2 - \bar{h}_1) - \frac{i\omega}{2} (1 - H) f' (\bar{h}_2 - \bar{h}_1) \\ &\quad + \frac{f^2}{2r^2} (\bar{h}_2 - \bar{h}_4) - \frac{f f'}{2r} (\bar{h}_1 - \bar{h}_5 - f \bar{h}_3 - 2f \bar{h}_6), \end{aligned} \quad (\text{A3})$$

$$\mathcal{M}_{3j}^{(0)} \bar{h}_j = -\frac{f}{2r^2} \left[\bar{h}_1 - \bar{h}_5 - \left(1 - \frac{4M}{r} \right) (\bar{h}_3 + \bar{h}_6) \right], \quad (\text{A4})$$

$$\mathcal{M}_{4j}^{(0)} \bar{h}_j = \frac{f f'}{4} \partial_r (\bar{h}_4 - \bar{h}_5) - \frac{i\omega (1 - H) f'}{4} (\bar{h}_4 - \bar{h}_5) - \frac{\lambda_1}{2} \frac{f}{r^2} \bar{h}_2 - \frac{f f'}{4r} (3\bar{h}_4 + 2\bar{h}_5 - \bar{h}_7 + \lambda_1 \bar{h}_6), \quad (\text{A5})$$

$$\mathcal{M}_{5j}^{(0)} \bar{h}_j = \frac{f}{r^2} \left[\left(1 - \frac{9M}{2r} \right) \bar{h}_5 - \frac{\lambda_1}{2} (\bar{h}_1 - f \bar{h}_3) + \frac{1}{2} \left(1 - \frac{3M}{r} \right) (\lambda_1 \bar{h}_6 - \bar{h}_7) \right], \quad (\text{A6})$$

$$\mathcal{M}_{6j}^{(0)} \bar{h}_j = -\frac{f}{2r^2} \left[\bar{h}_1 - \bar{h}_5 - \left(1 - \frac{4M}{r} \right) (\bar{h}_3 + \bar{h}_6) \right], \quad (\text{A7})$$

$$\mathcal{M}_{7j}^{(0)} \bar{h}_j = -\frac{f}{2r^2} (\bar{h}_7 + \lambda \bar{h}_5), \quad (\text{A8})$$

$$\mathcal{M}_{8j}^{(0)} \bar{h}_j = \frac{f f'}{4} \partial_r (\bar{h}_8 - \bar{h}_9) - \frac{i\omega (1 - H) f'}{4} (\bar{h}_8 - \bar{h}_9) - \frac{f f'}{4r} (3\bar{h}_8 + 2\bar{h}_9 - \bar{h}_{10}), \quad (\text{A9})$$

$$\mathcal{M}_{9j}^{(0)} \bar{h}_j = \frac{f}{r^2} \left(1 - \frac{9M}{2r} \right) \bar{h}_9 - \frac{f}{2r^2} \left(1 - \frac{3M}{r} \right) \bar{h}_{10}, \quad (\text{A10})$$

$$\mathcal{M}_{10j}^{(0)} \bar{h}_j = -\frac{f}{2r^2} (\bar{h}_{10} + \lambda \bar{h}_9). \quad (\text{A11})$$

In the matrix representation (69) of the field equations, these coupling terms appear in the form $-\frac{4}{f^2} \mathcal{M}_{ij}^{(0)} \bar{h}_j$, which we write explicitly in terms of (algebraic) matrices \mathcal{M}_h and $\mathcal{M}_{\partial h}$ acting on the vector ψ defined in Eq. (72) and its radial derivative $\partial_r \psi$. The matrix \mathcal{M}_h has the explicit form

$$\mathcal{M}_h = \frac{2}{r^2 f} \times \begin{pmatrix} -2(1 - \frac{9M}{2r}) & 1 - \frac{3M}{r} \\ \lambda & 1 \end{pmatrix} \quad (\text{A12})$$

for $\ell > 0$, $m > 0$ and $\ell + m$ odd;

$$\mathcal{M}_h = \frac{2}{r^2 f} \times \begin{pmatrix} -(1 - 4M/r) & f(1 - 4M/r) - 2iM\omega H & (1 - 4M/r) & f(1 - 6M/r) & 0 \\ 1 & -(1 - 4M/r) & -1 & -(1 - 4M/r) & 0 \\ \lambda_1 & -\lambda_1 f & -2(1 - 9M/(2r)) & -\lambda_1(1 - 3M/r) & (1 - 3M/r) \\ 1 & -(1 - 4M/r) & -1 & -(1 - 4M/r) & 0 \\ 0 & 0 & \lambda & 0 & 1 \end{pmatrix} \quad (\text{A13})$$

for $\ell > 0$, $m > 0$ and $\ell + m$ even; and the same matrix (A13) for $\ell = 1$, $m = 1$ but with the bottom row and rightmost column omitted.

The matrix $\mathcal{M}_{\partial h}$ in Eq. (73) has the form $\mathcal{M}_{\partial h} = \mathbf{0}_{2 \times 2}$ for $\ell > 0$, $m > 0$ and $\ell + m$ odd,

$$\mathcal{M}_{\partial h} = -\frac{4M}{r^2} \times \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad (\text{A14})$$

for $\ell > 0$, $m > 0$ and $\ell + m$ even; and the same matrix (A14) for $\ell = 1$, $m = 1$ but with the bottom row and rightmost column omitted.

Here we have only provided the explicit matrices for $\omega_m \neq 0$ cases. For $\omega_m = 0$, the gauge conditions (67) and (68) are used to eliminate \bar{h}_6 and \bar{h}_7 , reducing the dimensions of the matrices.

The matrix $\delta \mathcal{M}_h$ in Eqs. (244) is given explicitly as $\delta \mathcal{M}_h = \mathbf{0}_{2 \times 2}$ for $\ell > 0$, $m > 0$ and $\ell + m$ odd;

$$\delta \mathcal{M}_h = -\frac{4M}{r^2 f} i (\omega \delta H + \delta \omega H) \times \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad (\text{A15})$$

for $\ell > 0$, $m > 0$ and $\ell + m$ even; and

$$\delta \mathcal{M}_h = -\frac{4M}{r^2 f} i (\omega \delta H + \delta \omega H) \times \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (\text{A16})$$

for $\ell = 1$, $m = 1$.

Finally, the quantities $\mathcal{M}_{ij}^{(1)}$ appearing in the second-

order source via Eq. (65) are given by

$$\mathcal{M}_{1j}^{(1)} \bar{h}_j = -\frac{1}{2} f f' H \vec{\partial}_\nu \bar{h}_3, \quad (\text{A17a})$$

$$\mathcal{M}_{2j}^{(1)} \bar{h}_j = -\frac{f'}{2} \left[f H \vec{\partial}_\nu \bar{h}_3 - (1 - H) \vec{\partial}_\nu (\bar{h}_2 - \bar{h}_1) \right], \quad (\text{A17b})$$

$$\mathcal{M}_{4j}^{(1)} \bar{h}_j = \frac{f'}{4} (1 - H) \vec{\partial}_\nu (\bar{h}_4 - \bar{h}_5), \quad (\text{A17c})$$

$$\mathcal{M}_{8j}^{(1)} \bar{h}_j = \frac{f'}{4} (1 - H) \vec{\partial}_\nu (\bar{h}_8 - \bar{h}_9), \quad (\text{A17d})$$

$$\mathcal{M}_{ij}^{(1)} \bar{h}_j = 0 \quad \text{for } i = 3, 5, 6, 9, 10. \quad (\text{A17e})$$

2. Gauge conditions

The operators in the gauge conditions (67) and (68) are given by

$$\begin{aligned} Z_{1j}^{(0)} \bar{h}_j &= i\omega_m (\bar{h}_1 + f \bar{h}_3 + H \bar{h}_2) \\ &+ \frac{f}{r} (r \partial_r \bar{h}_2 + \bar{h}_2 - \bar{h}_4), \end{aligned} \quad (\text{A18a})$$

$$\begin{aligned} Z_{2j}^{(0)} \bar{h}_j &= i\omega_m (\bar{h}_2 + H \bar{h}_1 - H f \bar{h}_3) + f \left(\partial_r \bar{h}_1 - f \partial_r \bar{h}_3 \right. \\ &+ \left. \frac{1}{r} [\bar{h}_1 - \bar{h}_5 - f \bar{h}_3 - 2f \bar{h}_6] \right), \end{aligned} \quad (\text{A18b})$$

$$\begin{aligned} Z_{3j}^{(0)} \bar{h}_j &= i\omega_m (\bar{h}_4 + H \bar{h}_5) \\ &+ \frac{f}{r} [r \partial_r \bar{h}_5 + 2\bar{h}_5 + \ell(\ell + 1) \bar{h}_6 - \bar{h}_7], \end{aligned} \quad (\text{A18c})$$

$$\begin{aligned} Z_{4j}^{(0)} \bar{h}_j &= i\omega_m (\bar{h}_8 + H \bar{h}_9) \\ &+ \frac{f}{r} (r \partial_r \bar{h}_9 + 2\bar{h}_9 - \bar{h}_{10}), \end{aligned} \quad (\text{A18d})$$

and

$$Z_{1j}^{(1)} \bar{h}_j = -\bar{\partial}_V (\bar{h}_1 + f \bar{h}_3 + H \bar{h}_2), \quad (\text{A19a})$$

$$Z_{2j}^{(1)} \bar{h}_j = -\bar{\partial}_V (\bar{h}_2 + H \bar{h}_1 - f H \bar{h}_3), \quad (\text{A19b})$$

$$Z_{3j}^{(1)} \bar{h}_j = -\bar{\partial}_V (\bar{h}_4 + H \bar{h}_5), \quad (\text{A19c})$$

$$Z_{4j}^{(1)} \bar{h}_j = -\bar{\partial}_V (\bar{h}_8 + H \bar{h}_9). \quad (\text{A19d})$$

Appendix B: Basis of homogeneous solutions

1. Lorenz Gauge

Our method of variation of parameters requires the construction of a basis of homogeneous solutions, as described around Eq. (115). We obtain these basis solutions following Ref. [49], for example. Half the members of the basis are regular at \mathcal{I}^+ , and half are regular at \mathcal{H}^+ . We denote the former as $\psi_{\ell m}^{k+}$ and the latter as $\psi_{\ell m}^{k-}$ ($k = 1, \dots, d$). For $\omega_m \neq 0$ modes, each $\psi_{\ell m}^{k+}$ represents a purely outgoing wave behaving like $\sim e^{-i\omega u}$ for $r \rightarrow \infty$, and each $\psi_{\ell m}^{k-}$ represents a purely ingoing wave behaving like $\sim e^{-i\omega v}$ at $r = 2M$. There are a total of $2d$ basis solutions, where d is the dimension of the system, equal to the number of elements in the vector $\psi_{\ell m}$; see, e.g., the vectors in Eq. (72).

We construct this basis by first choosing some inner and outer boundaries r_{in} and r_{out} , setting them as close to $r = 2M$ and $r = \infty$ as is practicable. Concretely, r_{in} and r_{out} are chosen such that any change making r_{out} larger, or bringing r_{in} closer to $2M$, does not affect the first 16 significant digits of the numerical solution. For each ℓm mode, at each boundary, we construct a set of d boundary conditions, $\psi_{\ell m}^{k-}(r_{\text{in}})$ or $\psi_{\ell m}^{k+}(r_{\text{out}})$. For the nonstationary modes ($\omega_m \neq 0$), we use the expansions

$$\psi_{\ell m}^{k+}(r_{\text{out}}) = e^{i\omega_m[r_{\text{out}}^* - k(r^*)]} \sum_{n=0}^{n_{\text{max}}^+} a_{k,n} r_{\text{out}}^{-n}, \quad (\text{B1a})$$

$$\psi_{\ell m}^{k-}(r_{\text{in}}) = e^{-i\omega_m[r_{\text{in}}^* - k(r^*)]} \sum_{n=0}^{n_{\text{max}}^-} b_{k,n} (r_{\text{in}} - 2M)^n. \quad (\text{B1b})$$

For the stationary modes ($\omega_m = 0$), we use

$$\psi_{\ell 0}^{k+}(r_{\text{out}}) = \sum_{n=\ell}^{n_{\text{max}}^+} (a_{k,n} + \bar{a}_{k,n} \log r_{\text{out}}) r_{\text{out}}^{-n}, \quad (\text{B2a})$$

$$\psi_{\ell 0}^{k-}(r_{\text{in}}) = \sum_{n=0}^{n_{\text{max}}^-} b_{k,n} (r_{\text{in}} - 2M)^n. \quad (\text{B2b})$$

Both of these apply for a generic time function $s = t - k(r^*)$.

The coefficients here are d -dimensional column vectors. They are different for each ℓm and are determined from recurrence relations derived by substituting

the ansatzes (B1) and (B2) into the field equations. Recurrence relations for the Lorenz-gauge boundary conditions can be found in Appendix A of [49]. n_{max}^\pm is fixed by an accuracy requirement.

Once the boundary conditions $\psi_{\ell m}^{k+}(r_{\text{out}})$ and $\psi_{\ell m}^{k-}(r_{\text{in}})$ are determined, we find the basis solutions $\psi_{\ell m}^{k\pm}$ everywhere in the spacetime by integrating the homogeneous field equations inward from r_{out} or outward from r_{in} , as appropriate. We note that we need the inner and outer homogeneous solutions over the entire domain, not just at the particle, for the retarded integrals in the calculation of the r_0 derivative.

For our Lorenz-gauge calculations, we integrated the homogeneous equations using an 8th-order Runge-Kutta Prince-Dormand (RKPD) routine from the GNU Scientific Library (GSL) repositories [72]. This is an adaptive routine. In it we set the absolute accuracy goal (ϵ_{abs}) to 10^{-16} and the relative accuracy goal (ϵ_{rel}) to 10^{-14} . ϵ_{abs} and ϵ_{rel} were determined such that reducing them made no difference to our numerical results up to the 16th significant figure. We set the outer boundary to be $r_{\text{out}} = 10^4 M$, taking into account that moving the boundary further out did not change our results for the homogeneous solutions up to the 16th significant figure. From similar considerations the inner boundary needs to be $r_{\text{in}} = (2 + 10^{-8})M$ or closer to the horizon. The GSL routine cannot take us closer than $r_{\text{in}} = (2 + 10^{-5})M$ without severe computational burdens setting in, due to factors of $1/f$ in the differential equation. To obtain accurate data closer to the horizon we used a greater-than-machine-precision (GMP) routine for solving coupled differential equations, based on the C++ library of GMP variables and functions [73].

2. Teukolsky

To construct an appropriate basis of homogeneous solutions for the Teukolsky equation, one can follow the same procedure as Appendix B1 by prescribing boundary conditions at some finite radii r_{in} and r_{out} for the radiative modes. The boundary conditions can take the form of Eq. (B1) as an asymptotic series solution:

$$\psi_{\ell m}^+(r_{\text{out}}) = e^{i\omega_m[r_{\text{out}}^* - k(r^*)]} \sum_{n=0}^{n_{\text{max}}^+} a_n \frac{f(r_{\text{out}})^5}{(\omega r_{\text{out}})^n}, \quad (\text{B3a})$$

$$\psi_{\ell m}^-(r_{\text{in}}) = e^{-i\omega_m[r_{\text{in}}^* - k(r^*)]} \sum_{n=0}^{n_{\text{max}}^-} b_n r_{\text{in}} (r_{\text{in}} - 2M)^n. \quad (\text{B3b})$$

Substituting the ansatzes in Eqs. (B3a) and (B3b) into the field equation yields the following recursion relations

for the coefficients a_n and b_n :

$$a_n = \frac{i}{2(k-2s-1)} [(\ell+n-s-1)(\ell-n+s+2)a_{n-1} + 2M(n-2)\omega_m(n-s-2)a_{n-2}], \quad (\text{B4a})$$

$$b_n = \frac{1}{2Mn(n-s-4iM\omega_m)} [(\ell(\ell+1)-s(s+1) + 4iM\omega_m(2n-2s-1) + 2ns - n(n-1))b_{n-1} + 2i\omega_m(n-2s-1)b_{n-2}], \quad (\text{B4b})$$

where $a_{2s+1} = b_0 = 0$, and all of the remaining terms in the series expansion are determined by imposing $a_{n<2s+1} = 0$ and $b_{n<0} = 0$ respectively. Other similar asymptotic expansions for the hyperboloidal Teukolsky equation we have presented here have been derived in [55, 56].

We have validated these boundary conditions by comparing our solutions to the homogeneous solutions produced by the `Teukolsky` package of the `BHPToolkit`. Furthermore, we have compared numerical values of the expansions with boundary conditions used within the `Numerical Integration` module, which utilises the Mano, Suzuki, and Tagkasugi method [74, 75] of solving the Teukolsky equation.

The boundary conditions for the homogeneous solutions $\psi_{\ell m}^\pm$ are then used to construct homogeneous solutions over the entire domain from r_{in} to r_{out} . Similar to the Lorenz gauge homogeneous solutions, $\psi_{\ell m}^+$ is obtained by integrating inwards from r_{out} with the boundary condition Eq. (B3a) while $\psi_{\ell m}^-$ is found by integrating outwards from r_{in} using Eq. (B3b). In contrast to the Lorenz gauge homogeneous equations, we integrate the homogeneous Teukolsky equation with `Mathematica's NDSolve` routine. The use of `Mathematica` allows us to solve the homogeneous equation to beyond-machine precision, when such accuracy is necessary. We find setting $r_{\text{out}} = 10^4 M$ and $r_{\text{in}} = (2 + 10^{-5})M$ to be sufficient boundaries to obtain a similar absolute accuracy goal as the Lorenz gauge case we discussed previously.

Appendix C: Teukolsky source term

In this appendix we explicitly give expressions for the Teukolsky source utilised in our calculations in Sec. X as well as a brief summary of their derivation.

1. Kinnersley tetrad

Our calculations in the Teukolsky formalism use the Kinnersley tetrad [53]. In Schwarzschild coordinates, the

components of the Kinnersley tetrad are given by

$$l^\alpha = \frac{1}{f} [1, f, 0, 0], \quad (\text{C1})$$

$$n^\alpha = \frac{1}{2} [1, -f, 0, 0], \quad (\text{C2})$$

$$m^\alpha = \frac{1}{\sqrt{2}r} \left[0, 0, 1, \frac{i}{\sin\theta} \right], \quad (\text{C3})$$

$$\bar{m}^\alpha = \frac{1}{\sqrt{2}r} \left[0, 0, 1, -\frac{i}{\sin\theta} \right]. \quad (\text{C4})$$

The null vectors are constrained by the normalisation

$$l^\alpha n_\alpha = -m^\alpha \bar{m}_\alpha = -1, \quad (\text{C5})$$

with all other contractions between tetrad legs vanishing.

2. GHP operators

Our presentation uses the GHP formalism [76], which we briefly summarize here; we refer the reader to Sec. 4.1 of Ref. [2] for a detailed review. The central idea of the GHP formalism, in its modification of the Newman-Penrose formalism, is the introduction of the concepts of spin and boost weights. Under spin and boost transformations, the null vectors transform as

$$\begin{aligned} l^\alpha &\longrightarrow \zeta \bar{\zeta} l^\alpha, & n^\alpha &\longrightarrow \zeta^{-1} \bar{\zeta}^{-1} n^\alpha, \\ m^\alpha &\longrightarrow \zeta \bar{\zeta}^{-1} m^\alpha, & \bar{m}^\alpha &\longrightarrow \zeta^{-1} \bar{\zeta} \bar{m}^\alpha, \end{aligned} \quad (\text{C6})$$

where ζ is an arbitrary complex number. A GHP quantity, χ , is then labelled as type $\{p, q\}$ if under the transformation (C6), the quantity transforms as $\chi \longrightarrow \zeta^p \bar{\zeta}^q \chi$. The GHP weight of a quantity is denoted $\chi \doteq \{p, q\}$. One can relate the GHP weights p and q to the spin-weight s and boost-weight b via $s = (p - q)/2$ and $b = (p + q)/2$. For the tetrad legs, one can read off the following GHP weights:

$$\begin{aligned} l^\alpha &\doteq \{1, 1\}, & n^\alpha &\doteq \{-1, -1\}, \\ m^\alpha &\doteq \{1, -1\}, & \bar{m}^\alpha &\doteq \{-1, 1\}. \end{aligned} \quad (\text{C7})$$

From the definition (97), one can read off $\psi_4 \doteq \{-4, 0\}$.

The GHP derivative operators \mathbb{P} , \mathbb{P}' , \mathfrak{D} , and \mathfrak{D}' that appear in Eqs. (100) and (101) act on spin- and boost-weighted objects. In the Kinnersley tetrad, they are given by

$$\mathbb{P} = \frac{1}{f} \left(\frac{\partial}{\partial t} + f \frac{\partial}{\partial r} \right), \quad (\text{C8})$$

$$\mathbb{P}' = \frac{1}{2} \left(\frac{\partial}{\partial t} - f \frac{\partial}{\partial r} - \frac{2bM}{r^2} \right), \quad (\text{C9})$$

and

$$\mathfrak{D} = \frac{1}{\sqrt{2}r} \left(\frac{\partial}{\partial \theta} + i \csc\theta \frac{\partial}{\partial \phi} - s \cot\theta \right), \quad (\text{C10})$$

$$\mathfrak{D}' = \frac{1}{\sqrt{2}r} \left(\frac{\partial}{\partial \theta} - i \csc\theta \frac{\partial}{\partial \phi} + s \cot\theta \right). \quad (\text{C11})$$

When acting on a generic object of spin weight s and boost weight b , \mathbf{P} raises b by 1, and \mathbf{P}' lowers it by 1; \mathfrak{D} raises s by 1, and \mathfrak{D}' lowers it by 1. When acting on spin-weighted spherical harmonics in particular, \mathfrak{D} and \mathfrak{D}' act as spin-raising and lowering operators such that

$$\sqrt{2r} \mathfrak{D}({}_s Y_{\ell m}) = -[\ell(\ell+1) - s(s+1)]^{1/2} {}_{s+1} Y_{\ell m}, \quad (\text{C12})$$

$$\sqrt{2r} \mathfrak{D}'({}_s Y_{\ell m}) = [\ell(\ell+1) - s(s-1)]^{1/2} {}_{s-1} Y_{\ell m}. \quad (\text{C13})$$

3. Point particle source

At leading order in our multiscale expansion, the stress-energy tensor (6) for a particle on a quasicircular orbit reduces to

$$\varepsilon T_{(1,0)}^{\mu\nu} = \frac{\mu}{r^2} \frac{u_{(0)}^\mu u_{(0)}^\nu}{u_{(0)}^t} \delta(r-r_0) \delta(\theta-\pi/2) \delta(\phi-\phi_p). \quad (\text{C14})$$

We focus on the quasicircular case, but the computation of the Teukolsky source proceeds in a similar manner for more generic orbital configurations. We write the four-velocity of the particle in terms of the leading-order orbital energy and angular momentum, \mathcal{E}_0 and \mathcal{L}_0 , such that $u_\mu = (-\mathcal{E}_0, 0, 0, \mathcal{L}_0)$, with

$$\mathcal{E}_0 = \frac{f_0}{\sqrt{1-3M/r_0}}, \quad \mathcal{L}_0 = \frac{r_0 \sqrt{M}}{\sqrt{r_0-3M}}, \quad (\text{C15})$$

where $f_0 := 1 - 2M/r_0$.

To construct the source for the Teukolsky equation given in Eq. (105), we act on the stress-energy tensor with the operator in Eq. (101) before decomposing the

resulting expression into the basis of spin-weighted spherical harmonic and Fourier modes such that

$${}_s S_{\ell m} = -\frac{1}{2\pi} \int_0^{2\pi} d\phi_p e^{im\phi_p} \int d\Omega {}_s \bar{Y}_{\ell m} {}_s S, \quad (\text{C16})$$

where $d\Omega = \sin\theta d\theta d\phi$. Here we have given the expression for generic spin weight s . We see from the expression in Eq. (101) that, for $s = -2$, angular derivatives appear in the form of \mathfrak{D}' derivatives. These can be moved onto the spin-weighted harmonic in Eq. (C16) using $\int d\Omega {}_s \bar{Y}_{\ell m} \mathfrak{D}'_{s+1} \Psi = -\int d\Omega \mathfrak{D}'_s \bar{Y}_{\ell m} {}_{s+1} \Psi$ for any s and any spin-weighted object ${}_{s+1} \Psi$. We can then exploit the spin-raising and lowering properties of \mathfrak{D} using $\mathfrak{D}'_s \bar{Y}_{\ell m} = \bar{\mathfrak{D}}_s \bar{Y}_{\ell m}$ followed by Eq. (C12), reducing the angular integral to an integral against ${}_{s+1} \bar{Y}_{\ell m}$.

In Eq. (101), the point particle stress-energy tensor enters through its tetrad components. In the Kinnersley tetrad, the relevant projections of Eq. (C14) are

$$T_{nn}^{(1,0)} = \frac{M f_0^2 \delta(r-r_0)}{4r_0^2 \sqrt{1-3M/r_0}} \delta(\theta-\pi/2) \delta(\phi-\phi_p), \quad (\text{C17})$$

$$T_{n\bar{m}}^{(1,0)} = \frac{iM^{3/2} f_0 \delta(r-r_0)}{2\sqrt{2} r_0^2 \sqrt{r_0-3M}} \delta(\theta-\pi/2) \delta(\phi-\phi_p), \quad (\text{C18})$$

$$T_{\bar{m}\bar{m}}^{(1,0)} = -\frac{M^2 \delta(r-r_0)}{2r_0^3 \sqrt{1-3M/r_0}} \delta(\theta-\pi/2) \delta(\phi-\phi_p). \quad (\text{C19})$$

Here we have used the distributional identity

$$X(r) \delta(r-r_0) = X(r_0) \delta(r-r_0) \quad (\text{C20})$$

for smooth $X(r)$. The full first-order Teukolsky source term then has the form

$${}_s S_{\ell m}^{(1,0)} = {}_s S_{\ell m}^{(A)} + {}_s S_{\ell m}^{(B)} + {}_s S_{\ell m}^{(C)}, \quad (\text{C21})$$

where for $s = -2$,

$$-{}_2 S_{\ell m}^{(A)} = \pi r^4 \frac{M \sqrt{\lambda \lambda_1} f_0^2 {}_0 \bar{Y}_{\ell m}(\pi/2, 0)}{r_0^{3/2} \sqrt{r_0-3M}} \delta(r-r_0), \quad (\text{C22})$$

$$-{}_2 S_{\ell m}^{(B)} = -i\pi r^3 \frac{\sqrt{M^3 \lambda} f_0 {}_{-1} \bar{Y}_{\ell m}(\pi/2, 0)}{r_0^2 \sqrt{r_0-3M}} \left[(2M+r-2ir^2\omega_m-7r^2f) \delta(r-r_0) - 2r^2 f' \delta'(r-r_0) \right], \quad (\text{C23})$$

$$-{}_2 S_{\ell m}^{(C)} = \pi r^4 \frac{M^2 {}_{-2} \bar{Y}_{\ell m}(\pi/2, 0)}{r_0^{5/2} \sqrt{r_0-3M}} \left[(\omega_m(2iM+r^2\omega_m) - r^2 f(5f-6i\omega_m)) \delta(r-r_0) \right. \quad (\text{C24})$$

$$\left. - r^2 f((2i\omega_m+6f)\delta'(r-r_0) + f\delta''(r-r_0)) \right].$$

Here we have used the angular delta functions in Eqs. (C17)–(C19) to evaluate the angular integral in Eq. (C16) (after integrating by parts as explained below that equation). We have also used ${}_s \bar{Y}_{\ell m}(\pi/2, \phi_p) = {}_s \bar{Y}_{\ell m}(\pi/2, 0) e^{-im\phi_p}$ (for all s) to evaluate the integral

over ϕ_p .

Finally, to express the source terms in the form we use in our numerical worldtube calculations, we need to express ${}_s S_{\ell m}^{(1,0)}$ in the canonical form (254), in which every term takes the form $X(r_0) \delta^{(n)}(r-r_0)$, with all coeffi-

cients of radial delta functions evaluated at r_0 rather than r . To achieve this, we use the relation Eq. (C20) along with similar identities for higher derivatives of Dirac delta functions:

$$\begin{aligned} X(r)\delta'(r-r_0) &= X(r_0)\delta'(r-r_0) - X'(r_0)\delta(r-r_0), \\ X(r)\delta''(r-r_0) &= X(r_0)\delta''(r-r_0) - 2X'(r_0)\delta'(r-r_0) \\ &\quad + X''(r_0)\delta(r-r_0). \end{aligned} \quad (\text{C25})$$

After applying those identities, we find the coefficients in Eq. (254) are given by

$$\begin{aligned} J_{\text{PP}}^{(A)} &= -\frac{4\pi r_0^2}{f_0^3\sqrt{r_0}-3M} \left[f_0 \left(\sqrt{\lambda\lambda_1} r_0^{3/2} f_{00} \bar{Y}_{\ell m}(\pi/2, 0) - i\sqrt{M\lambda} r_0^2 {}_{-1}\bar{Y}_{\ell m}(\pi/2, 0) \left(r_0 f_0 (r_0(7+2i\omega_m) - 13) \right. \right. \right. \\ &\quad \left. \left. - 2M(7r_0 - 15) \right) \right) - M\sqrt{r_0} {}_{-2}\bar{Y}_{\ell m}(\pi/2, 0) \left(M(4M^2(r_0(5r_0 - 48) + 56) - 2Mr_0(ir_0\omega_m(6r_0 - 17) \right. \right. \\ &\quad \left. \left. - 10r_0(r_0 - 9) + 96) - r_0^3(r_0\omega_m(\omega_m - 6i) - 5r_0 + 14i\omega_m + 42) - 42r_0^2) \right) \right], \end{aligned} \quad (\text{C26})$$

$$J_{\text{PP}}^{(B)} = \frac{8i\pi M^{3/2} r_0^2}{f_0^2\sqrt{r_0}-3M} \left[\sqrt{\lambda} r_0^2 f_{0-1} \bar{Y}_{\ell m}(\pi/2, 0) - i\sqrt{Mr_0} {}_{-2}\bar{Y}_{\ell m}(\pi/2, 0) (2M + r_0 f_0(3r_0 - 7) + ir_0\omega_m) \right], \quad (\text{C27})$$

$$J_{\text{PP}}^{(C)} = \frac{4M^2\pi r_0^{9/2} {}_{-2}\bar{Y}_{\ell m}(\pi/2, 0)}{f_0\sqrt{r_0}-3M}. \quad (\text{C28})$$

The parametric derivatives with respect to r_0 are then given by

$$\begin{aligned} \delta J_{\text{PP}}^{(A)} &= \frac{2\pi}{\sqrt{Mr_0^{3/2}(r_0-3M)^{3/2}} f_0^4} \left[r_0^2 f_0 \left(\sqrt{\lambda\lambda_1} r_0^{3/2} f_{00} \bar{Y}_{\ell m}(\pi/2, 0) (4M(r_0 - 3M) + 3r_0 f_0(7M - 2r_0)) \right. \right. \\ &\quad \left. \left. - iM\sqrt{\lambda} {}_{-1}\bar{Y}_{\ell m}(\pi/2, 0) \left((24Mr_0^2 f_0^2(9 - 7r_0) + r_0^3 f_0(49r_0 - 60) + 12M^2(7r_0 - 18) \right. \right. \right. \\ &\quad \left. \left. + 4Mr_0(21 - 12ir_0\omega_m - 7r_0) + r_0^2(14ir_0\omega_m - 5) \right) + 8M(3M - r_0)(6M + r_0(2ir_0\omega_m - 1)) \right) \\ &\quad \left. + M\sqrt{Mr_0} {}_{-2}\bar{Y}_{\ell m}(\pi/2, 0) \left(12M(3M - r_0)(8M^2 + 6iMr_0^2 - r_0^4) + r_0^4 f_0(24M^2(M(12r_0 - 25) - 4r_0(r_0 - 2)) \right. \right. \right. \\ &\quad \left. \left. + 2iMr_0^2\omega_m(3M(24r_0 - 71) + 4r_0(17 - 6r_0)) + r_0^4\omega_m^2(27M - 8r_0) + r_0^2 f_0^2(4r_0(r_0(10r_0 - 63) + 42) \right. \right. \\ &\quad \left. \left. - 9M(r_0(15r_0 - 98) + 70)) + 6ir_0^2\omega_m(M(49 - 27r_0) + 2r_0(4r_0 - 7)) + 4M(3M(r_0(5r_0 - 57) + 60) \right. \right. \\ &\quad \left. \left. \left. + r_0^2(54 - 5r_0) - 54r_0) \right) \right) \right], \end{aligned} \quad (\text{C29})$$

$$\begin{aligned} \delta J_{\text{PP}}^{(B)} &= -\frac{4iM^{3/2}\pi}{r_0^3(r_0-3M)^{3/2} f_0^3} \left[\sqrt{\lambda} r_0^5 {}_{-1}\bar{Y}_{\ell m}(\pi/2, 0) (60M^2 - 42Mr_0 + 7r_0^2) \right. \\ &\quad \left. - i\sqrt{Mr_0} r_0^{7/2} {}_{-2}\bar{Y}_{\ell m}(\pi/2, 0) \left(M^3(864 - 396r_0) + 2r_0^3(4r_0(3 + i\omega_m)) + 2M^2r_0(3r_0(80 + 13i\omega_m)) \right. \right. \\ &\quad \left. \left. + 3Mr_0^2(117 - r_0(63 + 17i\omega_m)) \right) \right], \end{aligned} \quad (\text{C30})$$

$$\delta J_{\text{PP}}^{(C)} = \frac{2M^2\pi r_0^{5/2} {}_{-2}\bar{Y}_{\ell m}(\pi/2, 0)}{(r_0-3M)^{3/2} f_0^2} (66M^2 - 47Mr_0 + 8r_0^2). \quad (\text{C31})$$

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