Self-Consistent Modeling of Gravitational Theories beyond General Relativity

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The majority of extensions to general relativity (GR) display mathematical pathologies—higher derivatives, character change in equations that can be classified within partial differential equation theory, and even unclassifiable ones—that cause severe difficulties to study them, especially in dynamical regimes. We present here an approach that enables their consistent treatment and extraction of physical consequences. We illustrate this method in the context of single and merging black holes in a highly challenging beyond GR theory.

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Introduction.—The gravitational wave window provides exciting opportunities to further test general relativity (GR), e.g., [1]. Especially in the context of compact binary mergers, gravitational waves produced by the strongest gravitational fields in highly dynamical settings arguably represent the best regime to explore deviations from GR, e.g., [2].

Such effort, the ability to extract consequences and propel theory forward, rely on at least having some understanding of the characteristics of potential departures, to search and interpret outcomes [3].

Unfortunately, the majority of proposed beyond GR theories have, at a formal level, mathematical pathologies which makes their understanding in general scenarios difficult [4]. Such pathologies may include loss of uniqueness, a dynamical change of character in the equations of motion (e.g., from hyperbolic to elliptic) or, even worse, having equations of motion (EOM) of unknown mathematical type (e.g., [6–12]). This, combined with the need to use computational simulations to study the (nonlinear or dynamical) regime of interest, pose unique challenges. Of note is that the standard mathematical approach to analyze partial differential equations (PDEs) [13]—where the high-frequency limit is examined—cannot be applied as it is in such a regime that the problems alluded to arise. Further, such a regime is incompatible with the very assumptions made to formulate most GR extensions that rely on effective field theory (EFT) arguments [14]. We note similar issues arise in broader contexts, where problems of interest are described by (systems of) partial differential equations derived from EFT. For relativistic hydrodynamics and the studies of astrophysical systems as well as quark-gluon plasmas, which share analog mathematical problems (e.g., [15,16]). Faced with these issues, solid novel ideas must be pursued to understand potential solutions.

We report here on a technique to *fix* the underlying equations of motion to an extent to which the viability of a given theory can be assessed [17]. In particular, it allows exploring relevant theories within their regime of validity and, in particular, monitoring whether the dynamics keeps the solution within it for cases of interest. This technique, partially explored in toy models [19,20] and restricted settings (e.g., [21–23]), is here developed for the general, and demanding scenario, of compact binary mergers. This requires further considerations not arising in the previously simplified regimes. Specifically, we present the first self-consistent study of both single and binary black hole (BH) merger in the context of an EFT of gravity where corrections to GR come through high powers (naturally argued for) in the curvature tensor leading to EOM with *a priori* unclassifiable mathematical character.

We adopt the following notation: Greek letters $(\mu, \nu, \rho, \ldots)$ to denote full spacetime indices and Latin letters $(i, j, k, \ldots)$ for the spatial ones. We use the mostly plus metric signature, and set $c = 1$.

Focusing on a specific theory.—While we could take any of a plethora of proposed beyond GR theories—almost all sharing the problems alluded to earlier—; for definiteness here we consider a specific extension to GR derived naturally from EFT arguments [24]. In this approach, high energy (i.e., above the cutoff scale) degrees of freedom are integrated out, and their effects are effectively accounted for through higher order operators acting on the lower energy ones. For the case of gravitational interactions, in vacuum assuming parity symmetry, and accounting for the simplest contribution, such an approach yields under natural assumptions [25]:

$$I_{\mathrm{eff}} = \frac{1}{16\pi G}\int d^4x\sqrt{-g}\left(R - \frac{1}{\Lambda^6}\mathcal{C}^2 + \cdots\right), \qquad (1)$$

where $\mathcal{C} = R_{\alpha\beta\gamma\delta}R^{\alpha\beta\gamma\delta}$ and the coupling scale Λ has units of $[M_S]^{-1}$ for some scale M_S. The EOM are $G_{\mu\nu} = 8\epsilon H_{\mu\nu}$, with $G_{\mu\nu}$ the Einstein tensor, $\epsilon \equiv \Lambda^{-6}$ and

$$\begin{aligned} H_{\mu\nu} = \mathcal{C}\Big[&\Box R_{\mu\nu} - \frac{1}{2}\nabla_\mu\nabla_\nu R - \frac{1}{16}\mathcal{C}g_{\mu\nu} - R_{\mu\lambda}R^{\lambda}{}_{\nu} \\ &+ R^{\alpha\beta}R_{\mu\alpha\nu\beta} + \frac{1}{2}R_{\mu\sigma\rho\lambda}R_{\nu}{}^{\sigma\rho\lambda}\Big] \\ &+ 2(\nabla^\alpha\mathcal{C})[\nabla_\alpha R_{\mu\nu} - \nabla_{(\mu}R_{\nu)\alpha}] + R_{\mu}{}^{\alpha}{}_{\nu}{}^{\beta}\nabla_\alpha\nabla_\beta\mathcal{C}. \end{aligned} \quad (2)$$

$H_{\mu\nu}$ is covariantly conserved, since it is derived from an action possessing local diffeomorphism invariance.

In GR ($\epsilon = 0$) the resulting EOMs can be shown to define a hyperbolic, linearly degenerate, nonlinear, second order, PDE system of equations with constraints (e.g., [26]). With suitable coordinate conditions, characteristics are given by the light cones and do not cross—thus shocks or discontinuities cannot arise. The right-hand side, however, spoils all these considerations. Derivative operators higher than second order appear—which render the equations outside formal PDE classifications. *How is one to approach the study of this problem?* First, one can simplify somewhat the EOM by applying an order reduction and replace the Ricci tensor and the Ricci scalar. Since in this Letter we consider vacuum spacetimes $\mathrm{Ric} \sim \mathcal{O}(\epsilon)$, the contribution of the Ricci tensor to the rhs is $\mathcal{O}(\epsilon^2)$ and we can ignore it at the order that we are considering. We are left with the following EOM at $\mathcal{O}(\epsilon)$:

$$G_{\mu\nu} = \epsilon\left(4\mathcal{C}W_{\mu}{}^{\alpha\beta\gamma}W_{\nu\alpha\beta\gamma} - \frac{g_{\mu\nu}}{2}\mathcal{C}^2 + 8W_{\mu}{}^{\alpha}{}_{\nu}{}^{\beta}\nabla_\alpha\nabla_\beta\mathcal{C}\right), \quad (3)$$

where $W_{\alpha\beta\gamma\delta}$ is the Weyl tensor since $R_{\mu\nu\rho\sigma} = W_{\mu\nu\rho\sigma} + \mathcal{O}(\epsilon)$. Then, $\mathcal{C} = W_{\alpha\beta\gamma\delta}W^{\alpha\beta\gamma\delta}$. System (3), containing derivatives up to fourth order of the spacetime metric (in $\nabla_\alpha\nabla_\beta\mathcal{C}$), has no proper classification within PDE theory.

Motivated by the prototypical example discussed in the Supplemental Material [27], we *fix* the system (3) by introducing a new independent variable $\widehat{\mathcal{C}}$ instead of $\mathcal{C}$ above and add an equation for it in the following way:

$$(\partial_t^2 - 2\beta^i\partial_{ti} + \beta^i\beta^j\partial_{ij})\widehat{\mathcal{C}} = \frac{1}{\sigma}(\mathcal{C} - \widehat{\mathcal{C}} - \tau\partial_0\widehat{\mathcal{C}}), \quad (4)$$

where second time derivatives of the metric in the rhs are replaced—following a reduction of order strategy—using the zeroth order Einstein equations. The resulting EOMs have at most second-time derivatives and $\widehat{\mathcal{C}}$ is damped to the physical $\mathcal{C}$ on a timescale $\simeq\sigma/\tau$ (for our choices, up to $\simeq 10M_S$, which is shorter than any dynamical timescales in the system). As a result, beyond a length scale $\simeq\sigma^{1/2}$ (for our choices, up to $\simeq 0.2M_S$) the system reduces to the original one, while shorter ones are damped and controlled, and we can explore even shorter scales through suitable extrapolation of our results, as we discuss in the Supplemental Material [27]. The new variable $\widehat{\mathcal{C}}$, in essence, brings back (some of) the degree(s) of freedom integrated out to arrive to the EFT theory, in this case a massive scalar (see e.g., [12]) and our strategy defines a completion of the EFT. Notice the operator $\partial_0 \equiv \partial_t - \beta^i\partial i$ with the advection vector (corresponding to the shift vector in the $3+1$ decomposition) helps ensuring inflow towards the BH(s). That a single scalar suffices to controlling the whole system is related to it encoding the only contribution of higher derivatives and controlling it results in an overall effect ensuring high frequency modes are kept at bay. Depending on the structure in other theories, one might need to introduce further quantities (see, e.g., [22]). Nevertheless, the overall strategy remains unchanged.

Initial data.—We define initial data by a single (for the single BH case) or a superposition of boosted BHs as described in GR and dynamically "turn on" the coupling ϵ bringing it from 0 to the desired value with a quadratic function in a window $t \in [10, 30]M$. This allows the coordinate conditions to settle before incorporating GR deviations, inducing only smooth constraint violations (which are damped through the now standard use of constraint damping [35,36]) and by-passing the solution of initial data problem within the EFT theory, a task which in itself has received also limited formal and numerical attention. Again the presence of higher derivatives obscures the treatment [37].

For initial data in the single BH case, we use a boosted BH solution derived from the conformal transverse-traceless decomposition [39–41], which uses an approximate conformal factor solution to the Hamiltonian constraint, valid for small boosts. For the binary BHs, we adopt Bowen-York-type-of initial data [42] describing two superposed equal mass, boosted, nonspinning BHs in a quasicircular orbit. The individual masses are $m_i \approx 0.5M$, $i = 1$, 2, and the separation is $D \sim 12M$ (initial orbital frequency $\simeq 0.025/M$). The momenta are tuned so this binary is initially in quasicircular motion, and in GR it describes 12 orbits before merger (the initial BHs velocities are similar to those in the single boosted BH case).

Evolution.—We use the GRCHOMBO code [43,44] and the CCZ4 formulation of the Einstein equations [45] (see also [46]) which implements the system (3) (with $\mathcal{C} \to \widehat{\mathcal{C}}$)-(4) with a distributed adaptive mesh refinement capabilities, [47] using 6th order finite difference operators for the spatial derivatives and the method of lines for time integration through a Runge Kutta of 4th order [48]. We adopt a standard 1+log slicing condition for the lapse α and the Gamma-driver for the shift β^i, and adopt Sommerfeld boundary conditions at the outer boundaries. We redefine the damping parameter $\kappa_1 \to \kappa_1/\alpha$ to ensure that it remains active inside the apparent horizon (AH) [50]; we decrease the damping parameter in the shift condition as well as increase σ in (4) at large distances from the centre of the binary to ensure that no violation of the CFL condition arises due to grids becoming coarser with our explicit time-stepping strategy (e.g., [51]). Otherwise, the chosen values for the constraint damping, shift and lapse conditions are $\{\kappa_1 = 1, \kappa_2 = -0.8, \kappa_3 = 1, \alpha_2 = \alpha_3 = 1, \alpha_1 = 2, \eta_1 = 0.75, \eta_2 = 1/M\}$ ([43]) The additional evolution equation (4) is implemented in the obvious first order form. We treat the BHs interior as in [11], removing the role of correcting terms, achieving stable evolutions with unduly high resolution (see the Supplemental Material [27] for more details).

With the total ADM mass M of the system setting a scale, our domain for the boosted BH case corresponds to the quadrant $x \in [-L, L]$ and $y, z \in [0, L]$ as symmetry allows for restricting it. We adopt $L = 384M$ with a the coarsest grid spacing (for production runs) $\Delta = 2M$; we then add another 6 levels of refinement. For the BH binary case the computational domain, exploiting symmetries, is given by $x, y \in [-L, L]$ and $z \in [0, L]$. In this case we adopt, $L = 512M$ and coarsest grid spacing (for production runs) $\Delta = 4M$; we then add another 8 levels of refinement (for convergence tests we consider up to $\Delta = 8/3M$ and same number of refined levels). We monitor several informative quantities, in particular, a "tracking measure": $\mathcal{T}(C, \hat{C}) = [(||C - \hat{C}||_2)/(||C||_2)]$ and gravitational waves, which we extract at 6 equally spaced radii between $R = 50M$ and $R = 100M$ extrapolating the result to null infinity. In both cases we use the second (spatial) derivatives of the conformal factor [52] χ to estimate the local numerical error and determine whether a new refinement level needs to be added; in addition, we fix the spatial extent of certain levels to ensure the resolution at extraction radii is high enough. Lastly, we choose $|\epsilon| = 10^{-5} M_S^6$, which implies a coupling scale for new physics beyond GR of $\Lambda \approx 7/M_S \simeq 5M_\odot/M_S\ \mathrm{km}^{-1}$. Notice for this small scale, correction effects will be undoubtedly subtle, with a consequent high accuracy requirement to capture them. Here we undertake a first study mainly focused on demonstrating the ability of the method to control the system. We will concentrate on assessing this and obtaining a qualitative description of observed consequences. We consider both signs for ϵ, the negative case satisfies the constraints argued for in [53], the positive one also provided azimuthal numbers of the solution are not large, which is our case. We here choose a conservative scale $M_S = 10M_\odot$, i.e., somewhat below (but comparable) to the smallest curvature scale set by the masses of the individual BHs for all detected gravitational wave events. Choosing a smaller scale would imply that the modifications become $\mathcal{O}(1)$ during the inspiral [54] with arguably clear imprints on the observed signal, which is inconsistent with observations. Further, we note that it is natural to expect the scale to remain fixed, thus the larger the BH mass, the smaller the effect of corrections would be. This observation is particularly relevant as the BHs merge, as corrections after such regime would naturally become smaller [55]. We here focus on masses comparable to the length scale M_S, adopting individual BH masses $m_i = M_S/2 = 5M_\odot$.

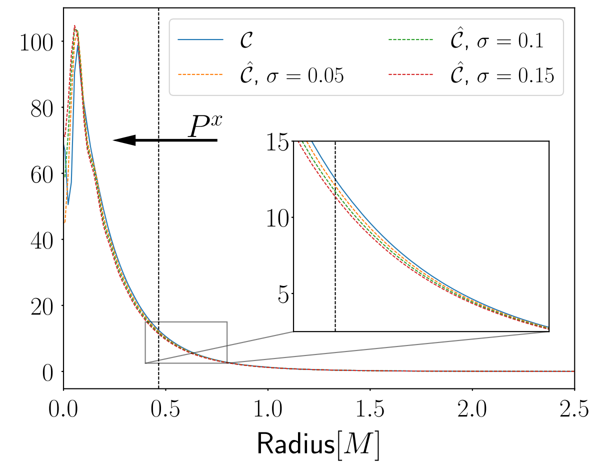

FIG. 1. $\mathcal{C}$ and $\hat{\mathcal{C}}$ on a line starting from the puncture and trailing the boosted BH—where differences in tracking are larger—(at $t = 75M$, when all transients related to gauge and initial data have passed) for a fixed value of $\tau = 0.005$. The BH has mass $M = 0.5$ and momentum $P^x = 0.08M$. The vertical dashed black line denotes the location of the AH and the arrow indicates the direction of motion of the BH.

Single boosted black holes.—We confirmed our strategy's ability to evolve boosted (and stationary) BHs, with the solution reaching a steady state behavior shortly after the corrections are fully turned on. The solution is smooth without inducing growth in high frequency modes or signs of instability. Beyond GR effects are naturally larger in the BH region. By comparing the value of $\widehat{\mathcal{C}}$ and $\mathcal{C}$ (see Fig. 1) we confirm the former tracks the physical one quite well and that lower values of $\{\sigma, \tau\}$ improve the tracking behavior (see Fig. S2). Importantly, examination of the relative difference between two values of $\widehat{\mathcal{C}}$ obtained with two different values of σ (and analogously with $\mathcal{C}$) indicates errors associated to the choice of this parameter do not severely accumulate, thus the solution is not degraded by strong secular effects (see Fig. S4 [27]). For instance, it would take $\approx 10^6 M$ for the relative error for Kretschmann scalar with $\sigma = 0.1$ and 0.05 to be of order $\mathcal{O}(1)$. Numerical instabilities develop for smaller values of σ around the excision region, well inside the AH; these instabilities are sensitive to the details of the excision—improving with resolution. This suggests other forms of excision would be more robust as σ is decreased (e.g., [21]). With a successful handling of correction effects in single, moving BHs, we turn next focus on the challenging setting of binary BH merger.

Black hole binary mergers.—The binary tightens due to emission of gravitational waves which radiate energy and angular momentum from the system. Figure 2 shows the gravitational wave strains for different values of ϵ and contrasts them with the corresponding one in GR. The solution is smooth, without any signs of instability

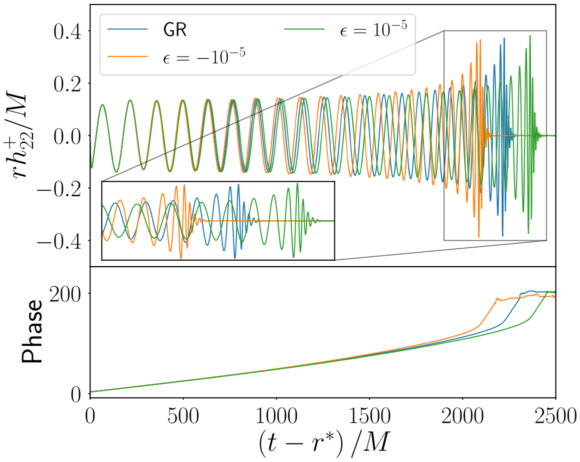

FIG. 2. Gravitational waves in GR and in the EFT theory ($\epsilon = \pm 10^{-5}$) with $\sigma = 0.0625$, $\tau = 0.005$. Top: $(\ell, m) = (2, 2)$ mode of the + polarization h^{+}_{22}, extrapolated to null infinity as a function of the retarded time $u = t - r^{*}$, where r^{*} is the tortoise radius. Bottom: gravitational wave phase of h_{22}.

throughout inspiral, merger, and ringdown. The corrections to GR and their high degree of nonlinearity and higher gradients contributions certainly tax resolution requirements. Our studies here are not focused on quantitatively sharp answers, but on testing the approach with enough resolution for qualitatively informative results and contrasting them with results in GR. In particular, we see that positive or negative values of ϵ induce a (slight) merger phase delay or advance. This is consistent with expectations, where BHs in this theory have nonzero tidal effects, encoded to leading order in the tidal love number $\kappa \propto \epsilon$ [58]. The binary behavior in the inspiral regime can be captured through a post-Newtonian analysis which shows tidal effects induce a phase offset $\propto -\kappa$ (hence $\propto -\epsilon$) [59] (see also [24,60]) for BHs with size comparable to M_S. Leading order post-Newtonian estimates for the phase difference give $\approx \pm 5 \times 10^{-3}$ radians up to a common gravitational wave frequency ($Mf = 0.01$) for negative or positive values of ϵ in Fig. 2. Our obtained offsets—extrapolated to $\sigma \to 0$—are consistent with the sign, though about 200 times larger (for a related study in Einstein-Scalar-Gauss Bonnet theory see Ref. [61]).

The BHs coalesce and the resulting peak strain is comparatively similar to that in GR and no significant further structure is induced in the multipolar decomposition of the waveforms, confirming that the solution stays within the EFT regime. Furthermore, the peak amplitude obtained with the BHs initially closer, so that merger takes place in only $\approx 200M$, agrees with the case taking $\approx 2000M$ to less than 1% relative difference. Moreover, since the merger gives rise to a BH with roughly twice the individual masses, corrections are reduced by $\approx 2^{-6}$. Thus the final BH is closer to a GR solution than the initial ones. After the peak amplitude, the system settles quickly to a stationary BH solution. This transition is described by an exponential, oscillatory behavior described by quasinormal modes (QNM).

While QNM spectra have only been computed for slowly rotating BHs in this theory [58,62], the departure observed in decay rates is consistent with extrapolation to higher spin values, though this is not the case in the oscillatory frequency. We note, however, that the extracted values for the case in GR, have relative errors $\approx 0.1\%$; since GR corrections to the QNMs in the case studied here are subleading by an order of magnitude such potential discrepancy can be attributed to a need for even higher accuracy to capture them sharply.

Also, as the solution approaches its final state we confirm it is axisymmetric. Such symmetry is expected in stationary BH solutions in EFTs of gravity [63]. By evaluating different scalars, such as the conformal factor χ of the spatial metric and $\widehat{\mathcal{C}}$, on the intersection of the AH (which in the stationary case coincides with the event horizon) with the equatorial plane, the tendency towards axisymmetry can be confirmed (Figs. S5–S6 [27]). Last, note that the difference in the innermost stable circular orbit frequency between slowly rotating BHs in this theory and GR goes as $\delta\Omega_{\mathrm{ISCO}} \propto -\epsilon$. Thus, extrapolating this observation to general spins, and following the successful strategy to estimate the final (dimensionless) spin in BH coalescence in GR [64], one can argue that the final BH spin should be higher or (lower) for positive or (negative) values of ϵ as the final "plunge" takes place with a higher or (lower) contribution of orbital angular momentum to the final BH. Cautioning that a higher accuracy is required to confirm this expectation, our results are consistent with it.

Discussion.—We demonstrated the ability of the "fixing" approach to enable studies of beyond GR theories. This approach, in particular, provides a practical way to explore phenomenology in the highly nonlinear and dynamical regime of compact binary mergers. Especially relevant is that it enables assessing whether the solution for cases of interest remains in the EFT regime and the impact of corrections in observable quantities. From this first analysis, we conclude the solution does remain in this regime for comparable mass, quasicircular mergers in the BH(s) exterior. Thus, much like in the case of GR, a strong UV energy flow takes place inside the horizon but not in the outside region, staying within the valid EFT regime. While in the current work we have focused on a specific theory and scale, our choice was motivated by stress-testing the approach with highly demanding challenges—brought by higher than second order derivatives and in the context of BH collisions. However, the underlying strategy is applicable also in beyond GR theories with second order equations that can induce change of character in the equation of motion (e.g., [8,22]). We note that for a particular class of nonlinear theories (with second order equations of motion) consistent, nonlinear studies have been presented [61,65,66]. However, they required significant supporting theoretical efforts to identify appropriate gauge conditions and merging BH solutions have been obtained up to some maximum coupling value otherwise mathematical pathologies arise. Our approach, in principle, provides a way to robustly explore beyond such coupling and, in general, study beyond GR theories self-consistently where such supporting theoretical input is not available or even achievable without strong—and *a priori* unjustifiable —assumptions [67]. Of course, practical application of the approach described here should be mindful of checking results upon variations of *ad hoc* parameters to ensure, given a coupling length, scales are sufficiently resolved.

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largely unaffected would be equally valid. The “fixed system” is amenable to numerical studies and, in particular, to examine whether the solution scenarios of interest remain within the EFT regime. This observation is analog to the one pointed out in [34] for the case of the relativistic Navier Stokes equations. In our present case, it is interesting to note controlling a single scalar suffices for this purpose.

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