Abstract

Construction of astrophysically realistic initial data remains a central problem when modelling the merger and eventual coalescence of binary black holes in numerical relativity. The objective of this paper is to provide astrophysically realistic freely specifiable initial data for binary black hole systems in numerical relativity, which are in agreement with post-Newtonian results. Following the approach taken by Blanchet [1], we propose a particular solution to the time-asymmetric constraint equations, which represent a system of two moving black holes, in the form of the standard conformal decomposition of the spatial metric and the extrinsic curvature. The solution for the spatial metric is given in symmetric tracefree form, as well as in Dirac coordinates. We show that the solution differs from the usual post-Newtonian metric up to the 2PN order by a coordinate transformation. In addition, the solutions, defined at every point of space, differ at second post-Newtonian order from the exact, conformally flat, Bowen-York solution of the constraints.

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I. INTRODUCTION

A. General Context

Construction of ‘astrophysically motivated’ initial data is of utmost importance in efforts directed towards simulating binary black hole (BBH) mergers. Such simulations are crucial for the detection and characterization of gravitational waves by the currently operational ground-based (e.g. LIGO, VIRGO, TAMA, GEO600), future advanced ground-based and space-based (e.g. LISA) laser interferometers. The sensitivity of the detectors is considerably increased by matched filtering of the observed signal with sets of the expected full waveform. At present, the entire inspiral and eventual coalescence of the two bodies is viewed in terms of three consecutive phases. The first and longest duration phase, the gradual ‘adiabatic’ inspiral, is modelled accurately by post-Newtonian (PN) methods and solved analytically to an accuracy of 3.5PN\(^1\) (in the equations of motion and gravitational flux respectively)\(^2\). When the PN approximation is assumed to be no longer valid, numerical relativity simulations are used at present to model the second phase of the plunge and coalescence of the two bodies \(^3,4,5,6\). After the two compact bodies have merged, the resulting single object enters the final ringdown phase \(^7,8,9,10,11,12,13,14,15,16,17,18,19,20\), modelled accurately using linear perturbation techniques of single black holes.

Recently, significant advances have been made in the numerical simulation of the strong-field merger phase \(^13,14,15,17,18,19,20\), in particular, in its dynamical evolution. The latter enables the accurate description of the BBH’s dynamical evolution and the extraction of an emitted gravitational wave signal. In this respect, ‘astrophysically realistic’ initial data with an appropriate gravitational wave content would help to ensure that the final extracted signal is as close as desirable to the emitted waveform. Note that the term ‘astrophysically motivated, or realistic, data’ refers to initial data sets that are constructed from spacetimes representing astrophysical BBHs, the merger of which current and future generation interferometers will be able to detect after several centuries or millennia of their inspiral. As noted in Section \(^13\) initial data sets used in early works have not taken into account the information about the inspiral and radiation content of BBH systems prior to merger.

\(^1\) The notation 1PN corresponds to the formal $\sim 1/c^2$ level in a post-Newtonian expansion with respect to the Newtonian acceleration and gravitational flux (where $c$ is the speed of light).
Initial data is given traditionally in the standard 3+1 formalism \[22\] and its construction is non-trivial. The problem lies in choosing physically meaningful initial data, amongst an infinitely large number of non-physical data choices, representing the BBHs. The most widely used methods to construct initial data, such as the Extrinsic Curvature (EC) \[23\] and Conformal Thin-Sandwich (CTS) \[24\], adopt conformal decompositions of both the spatial 3-metric and the extrinsic curvature. This results in a set of coupled elliptic partial differential equations, which are to be solved numerically under appropriate inner and outer boundary conditions, together with a set of freely specifiable parameters, referred to later in this paper as ‘free data’.

B. Related Work

For numerical convenience, early works \[25, 26\] devoted to constructing initial data sets for BBHs introduce a number of significant simplifying assumptions. These include conformal flatness, maximal slicing, together with the Bowen-York extrinsic curvature\[27\]. However, with considerable recent advances in spectral methods, as exemplified by \[28, 29, 30\], and finite element and finite difference techniques, limitations of numerical approaches are no longer seen as a serious obstacle. Moreover, several highly-developed 3D numerical software \[13, 14, 15, 17, 18, 19, 20\] for evolving black hole binaries already exist, enabling gravitational wave extraction. This makes it timely now to go beyond the initial assumptions of conformal flatness, maximal slicing and the use of the Bowen-York extrinsic curvature, and to provide astrophysically motivated initial data.

Among the more recent works that aim to overcome the limitations of the above assumptions, \[31, 32, 33\] use the alternative double superposed Kerr-Schild approach, \[34\] uses the PN method in ADM Transverse Traceless (ADMTT) coordinates, \[35, 36, 37\] use an asymptotic matching scheme, and \[28, 29, 38, 39\] develop helical-Killing vector/quasi-equilibrium initial data. These four approaches are briefly discussed below; the reader is referred to \[40\] and \[41\] for a more detailed discussion.

Taking the double superposed Kerr-Schild approach first, proposed initially in \[31\] and

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2 This is the analytical solution to the decoupled momentum constraint for a conformally flat spacetime and maximal hypersurface, was first given in \[27\], where it was checked by two surface integrals over a sphere at infinity.
developed further in [32, 33], it is important to note that Kerr spacetimes do not admit conformally flat slices. In this approach, the free data are constructed from a linear superposition of two single (spinning or boosted) black holes in Kerr-Schild coordinates representing the spatial conformal metric. Furthermore, the Kerr-Schild data advantageously reduce into stationary Kerr in the specific limit of two widely-separated black holes. The Kerr-Schild free data have also been numerically implemented [32] to obtain full initial data sets and are amongst the more extensively studied of all astrophysically motivated free data; see, for example, [42]. However, as this work notes (see Appendix A), the superposed Kerr-Schild initial data disagrees with post-Newtonian results at the second-post-Newtonian order.

In relation to PN free data, similar to Kerr spacetimes, binary black hole systems are also not conformally flat at second post-Newtonian order [43, 44]. It is widely acknowledged now that post-Newtonian results modelling the gradual inspiral should suggest a more astrophysically relevant form of the free data for the last few stable orbits prior to the Innermost Circular Orbit (ICO)\(^4\). This is an important motivation for our work, and has also been considered in the PN method in ADMTT coordinates [34].

The PN method in ADMTT coordinates due to Tichy et al. [34] proposes the direct adoption of the 2PN metric in ADM coordinates as the conformal spatial metric. The scheme outlined in [34] is for a numerically computed conformal factor to ‘correct’ the initial post-Newtonian solution and, thus, to account for higher-order post-Newtonian terms in the physical metric, which were initially neglected in the proposed conformal counterpart. The PN initial data in [34] are based on the PN results in the ADMTT gauge. Motivations given there for the choice of ADMTT gauge apply equally well to PN free data in the harmonic gauge, which is used in our work. Among these commonalities between the two methods, i.e. [34] and our work, firstly, both methods easily find expressions for the conformal 3-metric and extrinsic curvature without any logarithmic terms. Secondly, to the 1.5PN order \(\sim O(\frac{1}{c^3})\), the freely specifiable data sets due to both methods also agree with the puncture approach [26] and the choice in a specific hypersurface where the trace of the extrinsic curvature, \(K\),

\(^3\) These represent the solution, obtained numerically, to the coupled elliptic partial differential constraint equations using the freely specifiable parameters, or free data.

\(^4\) The ICO is defined by the minimum of the binary’s energy function for circular orbits. The definition does not include, significantly, radiation reaction terms and, therefore, is not physically meaningful in the context of exact radiative solutions. It is well-defined, however, for both numerical [28, 29] and 3PN calculations, and allows for comparisons between the two facilitating greater understanding.
(otherwise known as the ‘mean curvature’) vanishes. Finally, the two free data sets do not include, for the time being at least, any radiation content.

In the asymptotic matching scheme, following the initial work by Alvi [35], Yunes et al. [36, 37] propose an approximate metric for corotating BBHs spacetimes. Advantageously, this includes both 1PN effects, and, unlike in post-Newtonian free data sets due to Tichy et al. [34] discussed above and our work, tidal effects experienced by each black hole when close to one another. The metric is obtained by asymptotically matching a post-Newtonian metric for a binary system to a perturbed Schwarzschild metric modelling each black hole. At present, the method must be first projected onto the constraint hypersurface before numerical implementation. In addition, the method currently employs post-Newtonian results at the 1PN order, and considers the specific configuration of corotating BBHs.

Turning our attention to the fourth approach, that is, construction of helical-Killing vector/quasi-equilibrium initial data, Gourgoulhon et al. [28, 29] and Cook [39] first showed, by assuming an approximate helical-Killing vector for orbits prior to merger, a conformally flat spacetime and maximal slicing, that the four constraints plus one evolution equation simplify considerably in the CTS decomposition. The resulting set of equations is solvable numerically using spectral methods. Subtle problems, however, remain with the choice of inversion-symmetric inner boundary conditions at excision spheres around the singularities of the black holes - an implicit consequence of specifying a Misner topology. In this respect, Cook et al. [38] recently proposed other physically-motivated quasi-equilibrium boundary conditions, which allow for arbitrary specifications of the conformal metric, mean curvature, and the shape of the excision regions. As is mentioned later, helical-Killing vector/quasi-equilibrium initial data sets have been studied in detail through construction of quasi-circular orbits and in comparison with post-Newtonian work; see [45, 46] and [38, 47] respectively. An advantage over the double superposed Kerr-Schild method is that this approach does not require the specification of the extrinsic curvature. In addition, BBH dynamical evolutions have been performed recently for quasi-circular orbits. For example, [11] uses a scheme based on excision, new gauges, the BSSN formulation [48, 49, 50, 51], and a corotating frame, together with initial data constructed by means of the puncture method [26], whereas [52] uses the generalized harmonic evolution scheme [12, 13, 20] based on Cook-Pfeiffer initial data [38].

In contrast to the above methods, Blanchet [1] presents an alternative set of PN moti-
vated free data for the time-symmetric constraints, corresponding to two Schwarzschild black holes momentarily at rest\textsuperscript{5}. This work proposes a particular solution to the time-symmetric constraints in the form of the conformal metric, \(\tilde{\gamma}_{ij}\). The solution is such that the post-Newtonian expansion of the corresponding physical metric, \(\gamma_{ij}\), is isometric to the standard post-Newtonian metric in harmonic coordinates at 2PN order as \(c \to +\infty\). Furthermore, the solution is defined globally in space and differs from the Brill-Lindquist solution \textsuperscript{55} for conformally-flat spacetimes at 2PN. It is important to note that for the numerical implementations of BBH coalescence, the time-symmetric constraints involved relate to physically unrealistic events. This is because, from a general astrophysical perspective, black hole binaries prior to merger possess a velocity and, hence, impart a non-zero value to the extrinsic curvature to the hypersurface, i.e. \(K_{ij} \neq 0\), \(K_{ij}\) being the physical extrinsic curvature.

In this respect, our work aims to establish physically realistic free data for the plunge and merger phase of two black holes in numerical relativity, in conformity with post-Newtonian results \textsuperscript{56}. It follows from, and develops further, the time-symmetric approach proposed in \textsuperscript{1}.

Before entering into the details of our work, we remark on some of the difficulties in assessing how significant is the deviation arising from the assumption of a conformally flat metric for the merger of BBHs. Firstly, as shown by Pfeiffer \textit{et al.} \textsuperscript{42}, the resulting initial data sets are particularly sensitive to the choice in extrinsic curvature, as opposed to in the conformal 3-metric, \(\tilde{\gamma}_{ij}\). Their work is based on a comparison of initial data sets based on three different conformal decompositions of the initial constraints for BBHs. These initial data sets have been constructed by using both the double superposition of two black holes \textsuperscript{31, 32, 33} and the Bowen-York solution \textsuperscript{27}. Note that although the superposed Kerr-Schild data sets go beyond the standard assumption of conformal flatness,

\textsuperscript{5} The exact solutions of Misner \textsuperscript{53}, Lindquist \textsuperscript{54} and Brill and Lindquist \textsuperscript{55} to the time-symmetric constraints for conformally flat spacetimes provides an insight into the geometrostatic nature of two black holes, and in particular, into their topology: the solution for multiple black holes was directly inspired from the case of a single Schwarzschild black hole containing an Einstein-Rosen bridge (alternatively known as a ‘worm-hole’) joining two asymptotically flat universes. The Misner solution refers to two black holes, each containing an Einstein-Rosen bridge, which connects our universe to a second asymptotically flat region. In contrast, the Brill-Lindquist joins our universe to two distinct separate universes through two Einstein-Rosen bridges. Furthermore, it allows the computation at infinity of both the total ADM mass of the binary and each separate black hole, which then determines the gravitational binding energy of the system in the center of mass frame.
they disagree with post-Newtonian results at 2PN order (see Appendix A of this paper). Secondly, as is mentioned earlier, the recent results, in particular, the location of the ICO based on helical-Killing vector/quasi-equilibrium initial data \[28, 29, 38, 39\] for co-rotating and irrotational BBHs, show strong agreement with PN predictions \[38, 47\]. The agreement with PN results is not surprising, considering that helical symmetry is exact with respect to 2PN order. Despite encouraging agreement with post-Newtonian predictions, all the currently used quasi-equilibrium initial data sets assume ‘physically improbable’ conformally flat spacetimes.

C. An Overview of Our Contribution

In this work, we propose a particular solution in the form of conformal spatial metric, \(\tilde{\gamma}_{ij}\), and conformal extrinsic curvature, \(\tilde{K}_{ij}\), to the time-asymmetric constraint equations that represent a system of two moving black holes. The solution is chosen such that the post-Newtonian re-expansions of the corresponding physical metric, \(\gamma_{ij}\), and physical extrinsic curvature, \(K_{ij}\), are both isometric to the post-Newtonian metric in harmonic coordinates and post-Newtonian extrinsic curvature up to the 2PN order. Note that the post-Newtonian metric is formally valid in the source’s “near zone”\(^6\). Importantly for our work, it has also been proved that the post-Newtonian metric arises itself from the re-expansion of a “global” post-Minkowskian (expansion in G) multipolar solution as \(c \to \infty\), defined everywhere in spacetime, including the wave zone \([57]\). The solution for the conformal metric, \(\tilde{\gamma}_{ij}\), is given, firstly, in a symmetric trace-free form, similar to the approach instigated in \([1]\) and, secondly, for the first time, in Dirac coordinates. The motivation behind the choice of Dirac coordinates is to provide free data for constrained schema of the Einstein equations, such as the one based on a covariant generalized Dirac gauge\(^7\) and spherical coordinates, as proposed

\(^6\) The size of the near zone is much smaller than the characteristic gravitational wavelength.

\(^7\) As discussed in \([58]\), the advantages of implementing the covariant generalized Dirac gauge, defined as \([2.14]\) in \([58]\), are numerous. Firstly, it fully specifies the coordinates in the slice \(\Sigma_t\) (up to some inner boundary conditions for a slice containing holes); the latter property allows for the search for stationary solutions for the proposed set of equations, for instance, quasi–stationary initial conditions. In addition, the choice in gauge also results asymptotically in transverse–traceless (TT) coordinates, which are attractive for treating the problem of gravitational radiation and are analogous to the Coulomb gauge in electromagnetism. In addition, we show here that by relating our physical metric in Dirac coordinates, \(\gamma_{ij}^{Dirac}\), to the post-Newtonian metric, the resulting conformal factor \(\Psi^{DIRAC}\) assumes a simple form at
recently by Bonazzola et al. \cite{58}.

Furthermore, our PN free data is constructed in such a way that it is defined at every point in space and differs from the Bowen-York solution at 2PN order. By demonstrating equivalence relationships between our PN free data and the full 2PN metric, we also prove that the Bowen-York extrinsic curvature is physically equivalent to the 2PN derived extrinsic curvature. In detail, we show that each extrinsic curvature is defined with respect to a different hypersurface corresponding to a distinct 3+1 foliation of the full spacetime.

It is important to note that this work proposes only the freely specifiable parameters for initial data, hence, providing a free data scheme. The full physical initial data set is only possible after the constraint equations have been solved numerically, with appropriate inner and outer boundary conditions. Present numerical methods for generating a ‘constraint-satisfying’ data set from some physically motivated freely specifiable parameters include solving the constraints either using second-order finite difference techniques together with multigrid \cite{34} or successive over-relaxation \cite{32}, or using spectral methods \cite{28, 42}. Finite regions very close to the black hole singularities are frequently removed from the computational domain using standard excision techniques.

D. Structure of the Paper

The structure of the paper is as follows. Section \ref{sec:II} introduces the constraint equations in the 3+1 formalism required for presenting our approach and results. We outline the two standard conformal decompositions of the constraints: the Extrinsic Curvature (EC) and Conformal Thin Sandwich (CTS) methods, corresponding to a Hamiltonian or Lagrangian viewpoint of the problem respectively. In Section \ref{sec:III} we first present the proposed PN free data in both EC and CTS decompositions, namely \((\tilde{\gamma}_{ij}, \tilde{A}_{TT}^{ij}, K, \tilde{\sigma})\) and \((\tilde{\gamma}_{ij}, \tilde{u}^{ij}, K, \tilde{N} \text{ or } \partial_t K)\), respectively. Section \ref{sec:IV} subsequently outlines the proof of equivalence between our PN initial data and the full 2PN metric in harmonic coordinates, thus justifying the results given in Section \ref{sec:III}. We then briefly investigate the global properties of our proposed ‘near-zone’ PN solution and show that it is defined at every point in space. Based on our proofs, we finally show that the Bowen-York extrinsic curvature is physically equivalent to the 2PN derived curvature.\footnote{2PN order; see eqn. (4.17) in Section \ref{sec:IV}.}
extrinsic curvature. Section V concludes the paper with a summary of results.

II. 3+1 CONFORMAL DECOMPOSITION

The purpose of this section is to review the basic concepts related to the Extrinsic Curvature and Conformal Thin Sandwich decompositions of the constraints; this is necessary for the presentation of the results on PN free data in Section III. Our account here follows that in [40, 41], where more details may be found.

A. Preliminaries

In the Cauchy formalism of Einstein’s equations, a globally hyperbolic space-time is foliated into a set of space-like 3 dimensional hypersurfaces, Σₜ, where each slice is a constant hypersurface parameterized by the time coordinate t (t ∈ ℝ). According to the standard 3+1 decomposition, nₜ, a future-directed time-like unit normal to Σₜ, is defined as nₜ ≡ −N ∇ₜt, where N denotes the lapse function. Together with the causal stability of globally hyperbolic spacetimes, the global time vector field, t, is given by t = Nn + β, which is both transverse to Σₜ, and is normalized such that tαn = 1. The shift vector, β, thus trivially fulfills the condition βαn = 0. Following the definition of nₜ, the spacetime metric gₜν induces a purely spatial metric, γij, defined as γᵢⱼ = gᵢν + nᵢnᵢ, where subscripts in Latin and Greek characters denote three-dimensional and four-dimensional indices respectively.

The spacetime metric components, gᵢν, are thus expressed with respect to a preferred coordinate system (t, xᵢ) as,

\[ g_{\mu \nu} dx^\mu dx^\nu \equiv ds^2 = -N^2(dt)^2 + \gamma_{ij}(dx^i + \beta^i dt)(dx^j + \beta^j dt). \] (2.1)

Together with γᵢⱼ, a well-posed initial value problem must also specify how each spacelike hypersurface is embedded into the full spacetime. This is achieved by introducing the

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8 The lapse antidensity, α, a scalar of weight -1, is the undetermined multiplier of the scalar Hamiltonian constraint, which is in agreement with the canonical form of the ADM action. The relation between α and N is discussed later.
extrinsic curvature tensor, $K_{ij}$, i.e.,

$$K_{\mu\nu} \equiv -\frac{1}{2} \gamma_{\mu}^\rho \gamma_{\nu}^\sigma \mathcal{L}_n \gamma_{\rho\sigma}$$

or equivalently,

$$K_{ij} \equiv -\frac{1}{2} \mathcal{L}_n \gamma_{ij}, \quad (2.3)$$

where $\mathcal{L}_n$ represents the Lie derivative along the normal $n^\mu$ direction. By using the Gauss-Codazzi relations, the Einstein field equations are expressed in terms of six evolution equations,

$$\partial_t K_{ij} = N[\bar{R}_{ij} - 2K_i K^i_j + K K_{ij} - 8\pi G S_{ij} + 4\pi G \gamma_{ij} (S - \rho)] - \bar{\nabla}_i \bar{\nabla}_j N$$

$$+ \beta^i \bar{\nabla}_i K_{ij} + K_{il} \bar{\nabla}_j \beta^l + K_{jl} \bar{\nabla}_i \beta^l, \quad (2.4)$$

and four initial constraint equations,

$$\bar{R} + K^2 - K_{ij} K^{ij} = 16\pi G \rho, \quad (2.5)$$

$$\bar{\nabla}_j (K^{ij} - \gamma^{ij} K) = 8\pi G j^i, \quad (2.6)$$

where eqns. (2.5) and (2.6) are referred to as the Hamiltonian and momentum constraints respectively. In (2.4)-(2.6), $\rho$ denotes the matter energy density; $S_{ij}$ the matter stress tensor with $S \equiv S^i_i$, and $j^i$ the matter momentum density. In addition, $K \equiv K^i_i$ gives the trace of the extrinsic curvature, also known as the mean curvature, and $\bar{R}_{ij}$ is the 3-Ricci tensor associated with $\gamma_{ij}$. In order to avoid confusion, we follow the convention in [40] that covariant derivative and the Ricci tensor associated with the physical 3-metric $\gamma_{ij}$ are written with overbars as $\bar{\nabla}_j$ and $\bar{R}_{ij}$.

Definition (2.3) additionally results in a kinematic relation between $K_{ij}$ and $\gamma_{ij}$,

$$\partial_t \gamma_{ij} = -2N K_{ij} + \bar{\nabla}_i \beta_j + \bar{\nabla}_j \beta_i, \quad (2.7)$$

complementing the set of equations (2.4)-(2.6). Theoretically, the constraint equations are thus preserved exactly under evolution (due to the presence of the Bianchi identities).

Solutions to the most general form of the initial-value constraints for an extrinsic curvature $K_{ij} \neq 0$, as shown by equations (2.5), (2.6), are non-trivial, partly because the equations
do not fully specify\(^9\) the dynamical, constrained or gauge nature of the components of the 3-metric, \(\gamma_{ij}\), and extrinsic curvature, \(K_{ij}\). Moreover, it becomes even harder to find solutions to the constraints for the specific case of two black holes. Standard procedures to solve the initial-value problem adopt conformal decompositions of the metric and of the extrinsic curvature; see \[59, 60, 61, 62\].

The physical 3-metric, \(\gamma_{ij}\), is assumed to be conformally equivalent to a non-physical background metric, \(\tilde{\gamma}_{ij}\), by a conformal factor \(\Psi\), i.e.,

\[
\gamma_{ij} = \Psi^4 \tilde{\gamma}_{ij},
\]

where \(\Psi\) is the strictly positive background (conformal) factor.

The Hamiltonian constraint equation, (2.5), as first proposed by Lichnerowicz in \[60\], is thus re-expressed for a vacuum as,

\[
\tilde{\Delta} \Psi - \frac{1}{8} \Psi \tilde{R} - \frac{1}{8} \Psi^5 K^2 + \frac{1}{8} \Psi^5 K_{ij} K^{ij} = 0,
\]

where \(\tilde{\Delta} \equiv \tilde{\nabla}^i \tilde{\nabla}_i\) is the scalar Laplacian operator, and \(\tilde{\nabla}_j\) and \(\tilde{R}_{ij}\) are the covariant derivative and Ricci tensor associated with the conformal spatial metric, \(\tilde{\gamma}_{ij}\) (a tilde distinguishing, here and elsewhere, all quantities that have a conformal relationship with quantities in the physical space). A full conformal decomposition, however, requires introducing a conformal extrinsic curvature, \(\tilde{K}_{ij}\), as developed by York \[59\]. Our work concerns the two most widely used decompositions, which are seen to be consistent with each other: a) the fully conformally covariant EC decomposition, introduced recently in \[23\] and which improves on earlier non-conformally covariant decompositions, i.e. the Conformal Transverse Traceless (CTT) and Physical Transverse Traceless (PTT), and b) the CTS methods. Both methods involve expressing \(K_{ij}\) in terms of its trace and trace-free constituents,

\[
K_{ij} = A_{ij} + \frac{1}{3} \gamma_{ij} K.
\]

Each decomposition differs in its subsequent treatment of the symmetric trace-free extrinsic curvature, \(A_{ij}\). The EC method is based on the 3-metric, \(\gamma_{ij}\), and extrinsic curvature, \(K_{ij}\), where the latter is related uniquely to the canonical momentum, \(\pi^{ij}\). It provides a ‘Hamiltonian’ viewpoint to the conformal decomposition of the constraints; see \[41\]. In contrast, the

\(^9\) Constraints \(2.5\) and \(2.6\) restrict four out of the twelve degrees of freedom in \((\gamma_{ij}, K_{ij})\).
CTS decomposition considers the conformal metric, \( \tilde{\gamma}_{ij} \), and its time derivative, together with the mean curvature, \( K \), and the conformal lapse function, \( \tilde{N} \) (where, as discussed in Section II C, \( \tilde{N} \) is related to the time-derivative of \( K \) through a fifth coupled elliptic equation). It offers, therefore, a complementary ‘Lagrangian’ approach to the conformal decomposition of the initial data. The EC and CTS decompositions require a different set of free data, in particular, with respect to the extrinsic curvature or its tensor equivalent in the CTS instance. Both decompositions also result in, as illustrated in [42], different physical initial data. Sections II B and II C summarize the main results of the two decompositions.

B. Extrinsic Curvature Decomposition - Hamiltonian formalism

The extrinsic curvature method (see [23] for its proposed formulation and [41] for a detailed review) begins by applying a weighted transverse traceless decomposition to the tracefree extrinsic curvature, \( A_{ij} \), i.e.,

\[
A_{ij} = \frac{1}{\sigma}(\tilde{\Omega}X)^{ij} + A_{TT}^{ij},
\]

(2.11)

where \( A_{TT}^{ij} \) is a symmetric, tranverse-tracefree tensor and \( \sigma \) is a strictly positive and bounded function on the 3-dimensional hypersurface, \( \Sigma_t \), \( 0 < \epsilon \leq \sigma < \infty \) for \( \epsilon = constant \). Given the vector field, \( X^i \), the notation \( \tilde{\Omega} \) refers to the conformal longitudinal operator, \( (\tilde{\Omega}X)^{ij} \equiv \tilde{\nabla}^iX^j + \tilde{\nabla}^jX^i - 2\tilde{\gamma}^{ij}\tilde{\nabla}_lX^l \), satisfying \( (\tilde{\Omega}X)^{ij} = \Psi^{-4}(\tilde{\Omega}X)^{ij} \). Divergence of the symmetric trace-free tensor, \( A^{ij} \), results in the following expression\(^{10} \), \( \tilde{\nabla}_jA^{ij} = \tilde{\nabla}_j[\frac{1}{\sigma}(\tilde{\Omega}X)^{ij}] \), which can be solved for \( X^i \).

Having obtained \( A_{TT}^{ij} \) following the substitution of \( X^i \) in (2.11), the subsequent conformal scaling of \( A_{TT}^{ij} \equiv \Psi^{-10}\tilde{A}_{TT}^{ij} \) and \( \sigma \equiv \Psi^{6}\tilde{\sigma} \) allows for,

\[
A^{ij} = \Psi^{-10}\left(\tilde{A}_{TT}^{ij} + \frac{1}{\sigma}(\tilde{\Omega}X)^{ij}\right) = \Psi^{-10}\tilde{A}^{ij},
\]

(2.12)

\(^{10} \) It involves the well-defined elliptic operator in divergence form, \( \tilde{\nabla}_j[\sigma^{-1}(\tilde{\Omega})^{ij}] \), as discussed in [23] and [41]. For \( \sigma = 1 \), the latter operator reduces to the vector Laplacian, \( (\tilde{\Delta}Y)^{ij} \equiv \tilde{\nabla}_j(\tilde{\Omega}X)^{ij} \). As discussed in [23], this is solvable on compact and on asymptotically flat manifolds, given certain asymptotic conditions ([59] demonstrates the existence and uniqueness of a solution to (2.11) for closed manifolds). In the case of non-compact manifolds without boundaries, boundary conditions must always be specified and their choice will directly affect the solution of \( X^i \). As remarked in [23], there is no uniqueness property without boundary conditions.
where the weighted transverse trace-free decomposition in conformal space is \( \tilde{A}^{ij} \equiv \tilde{A}_{TT}^{ij} + \frac{1}{\bar{\sigma}} \left( (\tilde{\nabla} X)^{ij} \right) \).

Introduction of the weight function \( \sigma \) in [23] ensures that the extrinsic curvature decomposition commutes with conformal transformations of the free data\(^{11}\). Such a specific choice in the conformal scaling of \( \sigma \) also allows \( \sigma \) to be related directly to the lapse function, \( N \). As discussed in Section II C the conformal \( \tilde{N} \) is a component of the free data in the CTS decomposition.

In conjunction with \( \bar{\nabla}_j (\Psi^{-10} \tilde{S}^{ij}) = \Psi^{-10} \bar{\nabla}_j \tilde{S}^{ij} \), the complete set of elliptic constraint equations for a vacuum are,

\[
\bar{\nabla}_j \left( \frac{1}{\sigma} (\tilde{\nabla} X)^{ij} \right) - \frac{2}{3} \Psi^6 \bar{\nabla}^i K = 0, \tag{2.13}
\]

\[
\ddot{\tilde{\nabla}} \Psi - \frac{1}{8} \Psi \ddot{R} - \frac{1}{12} \Psi^5 K^2 + \frac{1}{8} \Psi^{-7} \tilde{A}_{ij} \tilde{A}^{ij} = 0. \tag{2.14}
\]

In this case, the set of free data comprises \((\tilde{\gamma}^{ij}, \tilde{A}_{TT}^{ij}, K, \bar{\sigma})\), which enables the solution to (2.13) and (2.14) for \( \Psi \) and \( X^i \) with appropriate inner and outer boundary conditions. Hence, given relationships (2.8), (2.10), \( A^{ij}_{TT} \equiv \Psi^{-10} \tilde{A}_{TT}^{ij} \), and \( \tilde{A}^{ij} \equiv \tilde{A}_{TT}^{ij} + \frac{1}{\bar{\sigma}} \left( (\tilde{\nabla} X)^{ij} \right) \), it is possible to construct the physical initial data, \( \gamma^{ij} \) and \( K_{ij} \).

C. Conformal Thin Sandwich (CTS) Decomposition - Lagrangian formalism

Instead of directly treating the extrinsic curvature itself (as in Section IIB), the CTS decomposition [24] considers the evolution of the metric between two neighboring hypersurfaces\(^{12}\). This is achieved by introducing the time-derivative of the conformal 3-metric, \( \ddot{\bar{u}}^{ij} \),

\[
\ddot{\bar{u}}^{ij} \equiv \partial_t \tilde{\gamma}^{ij}, \tag{2.15}
\]

\( \tilde{\gamma}^{ij} \) defined in (2.8), such that

\[
u^{ij} \equiv \gamma^{1/3} \partial_t (\gamma^{-1/3} \tilde{\gamma}^{ij}) \quad \text{and} \quad \ddot{\tilde{\gamma}}^{ij} \ddot{u}^{ij} \equiv 0^{13}.\]

Using a nontrivial conformal rescaling of both the lapse\(^{14}\), \( N \equiv \Psi^6 \tilde{N} \), and the tracefree extrinsic curvature,

---

\(^{11}\) This is in contrast to its earlier variants (i.e. the CTT and PTT decompositions), where the conformal transformation and transverse-traceless decomposition are non-commutative operations.

\(^{12}\) Advantageously, the method enables an understanding into the gauge choice and its subsequent evolution through the kinematic variables, \( N \) and \( \beta^i \).

\(^{13}\) This relationship allows for the conformal metrics on both hypersurfaces to have the same determinant to first order in \( \delta t \).

\(^{14}\) This scaling is a direct consequence of the conformal invariance of the lapse antdensity \( \alpha \), such that \( \ddot{\alpha} = \alpha \), where \( \alpha \) and \( \beta^i \) are undetermined multipliers of the constraints. When the scalar constraint is
\( A_{ij} \equiv \Psi^{-2} \tilde{A}_{ij} \), the kinematic relation (2.7) simplifies to,

\[
A^{ij} = \Psi^{-10} \tilde{A}^{ij} \equiv \frac{\Psi^{-10}}{2N} \left( (\tilde{L}\beta)^{ij} - \tilde{u}^{ij} \right).
\]  

(2.16)

Equation (2.16) implies form invariance under conformal transformations. In summary, the constraint equations assume the following form in the CTS decomposition,

\[
\nabla_j \left( \frac{1}{2N}(\tilde{L}\beta)^{ij} \right) - \nabla_j \left( \frac{1}{2N}\tilde{u}^{ij} \right) - \frac{2}{3}\Psi^6 \nabla_i K = 0
\]

(2.17)

\[
\tilde{A}\Psi - \frac{1}{8}\Psi \tilde{R} - \frac{1}{12}\Psi^5 K^2 + \frac{1}{8}\Psi^{-7} \tilde{A}_{ij} \tilde{A}^{ij} = 0
\]

(2.18)

The set of free data in this case are \((\tilde{\gamma}_{ij}, \tilde{u}^{ij}, K, \tilde{N})\). They solve for the constrained variables, \(\Psi\) and \(\beta^i\), in (2.17) and (2.18), under appropriate inner and outer boundary conditions. Thus, the physical initial values, \(\gamma_{ij}\) and \(K_{ij}\), follow in a straightforward manner.

We note that in practical computations, the set of four constraint equations in the CTS decomposition is often complemented by a fifth coupled elliptical equation relating the conformal lapse, \(\tilde{N}\), to the time derivative of the mean curvature, \(\partial_t K\). By eliminating \(R\) from the trace of (2.4) with (2.5) for a vacuum and after re-expressing the result in terms of their conformal counterparts, we obtain,

\[
\tilde{\Delta}(\tilde{N}\Psi^7) - (\tilde{N}\Psi^7) \left[ \frac{1}{8}\tilde{R} + \frac{5}{12}\Psi^4 K^2 + \frac{7}{8}\Psi^{-8} \tilde{A}_{ij} \tilde{A}^{ij} \right] = -\Psi^5 (\partial_t K - \beta^k \partial_k K),
\]

(2.19)

or alternatively,

\[
\tilde{\Delta} \tilde{N} + 14 \nabla^i \ln \Psi \tilde{\nabla}_i \tilde{N} + \tilde{N} \left[ \frac{3}{4}\tilde{R} + \frac{1}{6}\Psi^4 K^2 - \frac{7}{4}\Psi^{-8} \tilde{A}_{ij} \tilde{A}^{ij} + 42 \tilde{\nabla}_i \ln \Psi \tilde{\nabla}^i \ln \Psi \right] = -\Psi^{-2} (\partial_t K - \beta^k \partial_k K).
\]

(2.20)

The free data, therefore, consists solely of pairs of variables and their corresponding velocities, \((\tilde{\gamma}_{ij}, \tilde{u}^{ij}, K, \partial_t K)\), which is more in line with the Lagrangian approach of the CTS decomposition than using \((\tilde{\gamma}_{ij}, \tilde{u}^{ij}, K, \tilde{N})\) [41]. An additional motivation for extending the system of constraint equations\(^{15}\) is due to the natural choice of \(\partial_t K = 0\) in practical computations of quasi-equilibrium binary black initial data [28, 29, 38, 39]. In Section III B we satisfied, the ADM action results in the relationship \(\alpha = \tilde{N}\tilde{\gamma}^{-1/2}\), and therefore, \(N \equiv \Psi^6 \tilde{N}\) is obtained.\(^{14}\) Despite its frequent application, uniqueness and existence proofs do not exist at present for the extended CTS set of equations. Pfeiffer et al. [63] recently investigated the uniqueness properties of the extended CTS system though without reaching any firm conclusion. Two distinct solutions for the same free data based on linearized quadruple gravitational waves [64] were found in the extended system. For a given physical (conformally scaled) amplitude of the perturbation, the solution for the physical initial data, \(\gamma_{ij}\) and \(K_{ij}\), appears to be unique.
present the free data for both the simple and extended CTS formulations, using $\tilde{N}$ and $\partial_t K$ respectively.

**D. Correspondence between the weight function $\sigma$ and lapse function $N$**

The EC and CTS formalism are equivalent to each other for the specific choice of $\sigma = 2N$ and $\bar{\sigma} = 2\tilde{N}$. Such an equivalence relationship becomes possible following the introduction of the weight function, $\sigma$, and by specifying the particular conformal scaling, $\sigma \equiv \Psi^6 \bar{\sigma}$, in the EC decomposition; see [23, 41] for details.

Let us assume a stationary solution to Einstein’s equations with timelike Killing vector $l$ such that $\partial_t g_{ij} = 0$. As [23, 41] details, $\tilde{A}_{TT}^{ij}$ then vanishes for stationary spacetimes in the case $\sigma = 2N$ and $\bar{\sigma} = 2\tilde{N}$ in the EC decomposition, where $\tilde{A}_{TT}^{ij}$ is usually identified with the radiative degrees of freedom. This is generally not the case for stationary, non-static spacetimes in the previous CTT and PTT decompositions, which do not include the weight function, $\sigma$. Note that the standard Bowen-York free data specifies $\tilde{A}_{TT}^{ij} = 0$; see [27]. Alternatively, let us instead examine the particular choice $\bar{\sigma} = 1$, corresponding to the CTT decomposition\(^{16}\), in the case $\sigma = 2N$ and $\bar{\sigma} = 2\tilde{N}$.

In this work, we consider both specific instances; firstly, $\sigma = 2N$ and $\bar{\sigma} = 2\tilde{N}$ and, secondly, $\bar{\sigma} = 1$ (with no assumed relationship between $\sigma$ and $N$). The second case corresponds to the former CTT decomposition.

**III. POST-NEWTONIAN FREE DATA**

This section presents the proposed free data, namely, $(\tilde{\gamma}_{ij}, \tilde{A}_{TT}^{ij}, K, \tilde{\sigma})$ and $(\tilde{\gamma}_{ij}, \tilde{u}_{ij}^{\hat{b}}, K, \tilde{N} \text{ or } \partial_t K)$, based on post-Newtonian results at 2PN in EC (Hamiltonian) and CTS (Lagrangian) decompositions respectively. These have been introduced in Sections II.B and II.C respectively. We return in Section IV to present our reasoning behind the choice of the specific form of each of the components in the above free data.

As discussed in Section I, the EC and CTS methods offer two different perspectives in

\(^{16}\) Recall that the CTT decomposition is frequently used when solving the standard Bowen-York initial data and is a special case within the overall EC decomposition; see [4].
describing how each 3-spatial hypersurface is embedded in the full space-time\textsuperscript{17}, but do not differ in their definitions of the conformal spatial metric, $\tilde{\gamma}_{ij}$. Hence, the form of proposed conformal metrics, $\tilde{\gamma}_{ij}$, are, as expected, identical in both decompositions.

\section*{A. EC Decomposition}

We now present each of the components in the free data ($\tilde{\gamma}_{ij}, \tilde{\mathcal{A}}_{TT}^{ij}, K, \tilde{\sigma}$).

1. **Conformal metric: $\tilde{\gamma}_{ij}$**

Two possible options for the form of the conformal metric, $\tilde{\gamma}_{ij}$, are:

(a) **Symmetric-Traceless Form: $\tilde{\gamma}_{ij}$**

In this case, $\tilde{\gamma}_{ij}$ assumes the form

$$
\tilde{\gamma}_{ij} = \delta_{ij} - \frac{8G^2 m_1 m_2}{c^4} \frac{\partial^2 g}{\partial y_1^i \partial y_2^j} + \frac{4Gm_1}{c^4 r_1} v_1^i v_1^j + \frac{4Gm_2}{c^4 r_2} v_2^i v_2^j,
$$

where $m_1$ and $m_2$ refer to each of the two point particle masses respectively\textsuperscript{18}, i.e. the black hole masses in our model, $y_1$ and $y_2$ denote the black hole positions, $r_1 = |x - y_1|$ and $r_2 = |x - y_2|$ represent the distances to the black holes from the field point $x$, and $r_{12} = |y_1 - y_2|$ gives the distance between the black holes. In addition, $v_1 = dy_1/dt$ and $v_2 = dy_2/dt$ refer to coordinate velocities of the black holes. The term $\frac{\partial^2 g}{\partial y_1^i \partial y_2^j}$ comprises all the velocity-independent terms in (3.1) and represents the symmetric and tracefree (STF) projection\textsuperscript{19} of the double derivative of the function $g$ with respect to $y_1$ and $y_2$ respectively. The function $g$ first emerged as an elementary ‘kernel’ for the post-Newtonian direct iterative works \textsuperscript{56, 67} and is defined by,

$$
g(x; y_1, y_2) = \ln(r_1 + r_2 + r_{12}).
$$

\textsuperscript{17} In particular, the CTS method offers insights into the dynamics of the spacetime.

\textsuperscript{18} The ‘post-Newtonian’ masses, $m_1$ and $m_2$, are introduced in the post-Newtonian iteration as the coefficients of Dirac delta functions in the Newtonian density of point-like particles. They were shown in \textsuperscript{1} to agree with the ‘geometrostatic’ masses associated with the Brill-Lindquist solution in the time-symmetric instance.

\textsuperscript{19} i.e. $Q_{<ij>} = \frac{1}{2}(Q_{ij} + Q_{ji}) - \frac{1}{4}\delta_{ij}Q_{kk}$. 
It satisfies the Poisson equation in a complete distributional sense such that,

$$\Delta g = \frac{1}{r_1 r_2},$$  \hfill (3.3)

where $\Delta$ represents the standard flat-space Laplacian with respect to the field point $x$. The explicit expression for $i g_j$ is, therefore, given by,

$$i g_j \equiv \partial^2 g / \partial y^i_1 \partial y^j_2 = \frac{n^i_{12} n^j_{12} - \delta^i j}{r_{12}(r_1 + r_2 + r_{12})} + \frac{(n^i_{12} - n^i_1)(n^j_{12} + n^j_2)}{(r_1 + r_2 + r_{12})^2},$$  \hfill (3.4)

where the notations $n_1 = (x - y_1)/r_1$ and $n_2 = (x - y_2)/r_2$ refer to unit displacement vectors from $x$ to the black holes, and $n_{12} = (y_1 - y_2)/r_{12}$ is the unit displacement from black hole 1 to 2. We henceforth follow the notation introduced by the post-Newtonian works \[56, 65, 66, 67\], where $i g_j \equiv \partial^2 g / \partial y^i_1 \partial y^j_2$, \hfill (3.1) may be re-expressed in a fully expanded form as,

$$\tilde{\gamma}_{ij} = \delta_{ij} - \frac{8 G^2 m_1 m_2}{c^4} \left[ \frac{n^{<i}_{12} n^{>}_{12}}{r_{12}(r_1 + r_2 + r_{12})} + \frac{(n^{<i}_{12} - n^{<i}_1)(n^{>}_{12} + n^{>}_{2})}{(r_1 + r_2 + r_{12})^2} \right] + \frac{4 G m_1}{c^4 r_1} v^{<i}_1 v^{>}_1 + \frac{4 G m_2}{c^4 r_2} v^{<i}_2 v^{>}_2. \hfill (3.5)$$

The precise form of (3.1) is chosen such that the post-Newtonian expansion (when $c \to \infty$) of its corresponding physical metric $\gamma_{ij}$ is physically equivalent to the standard post-Newtonian spatial metric in harmonic coordinates \hfill [56] at 2PN order modulo a coordinate transformation. Such equivalence statements are detailed fully in Sections \hfill [IV A] and \hfill [IV B]. In addition, (3.1) is a component of the free data set $(\tilde{\gamma}_{ij}, \tilde{A}^{ij}_{TT}, K, \tilde{\sigma})$. As shown in Section \hfill [IV C], this free data set refers to a solution, albeit approximately, to the constraints which differs from the global conformally-flat Bowen-York solution \hfill [27] at second post-Newtonian order.

(b) **Dirac Coordinates**

Confining ourselves now to Dirac coordinates, the post-Newtonian derived conformal
metric, $\tilde{\gamma}_{ij}^{Dirac}$, takes the form\(^{20}\),
\[
\tilde{\gamma}_{ij}^{Dirac} = \delta_{ij} - \frac{8G^2m_1m_2}{c^4} [_{i}g_{j}]^{TT} + \left[ \frac{4Gm_1}{c^4r_1} v_i^j v_1^j \right]^{TT} + \left[ \frac{4Gm_2}{c^4r_2} v_2^j v_2^j \right]^{TT}, \tag{3.7}
\]
where the term $[_{i}g_{j}]^{TT}$ denotes the transverse–traceless form of the double derivative of the function $g$ \((3.2)\), with respect to $y_1$ and $y_2$ respectively. The explicit expression of $[_{i}g_{j}]^{TT}$ in \((3.7)\) is
\[
[_{i}g_{j}]^{TT} = (ig_{j}) + \frac{7}{8} \partial_{ij}g - \frac{3}{16} \partial_{ij} \left( \frac{r_1 + r_2}{r_{12}} \right) + \frac{1}{8} \partial_{ij} \left( \frac{r_1 - r_2}{r_{12}} \right) + \frac{1}{96} \partial_{ij} D \left( \frac{r_1^2 + r_2^2}{r_{12}} \right), \tag{3.8}
\]
where we refer to the notation used in \cite{1, 56} for $D \equiv \frac{\partial^2}{\partial y_1 \partial y_2}$, and the expressions subsequently derivable,
\[
Dg = \frac{1}{2r_1r_2} - \frac{1}{2r_1r_{12}} - \frac{1}{2r_2r_{12}}, \tag{3.9}
\]
\[
\partial_{ij} \left( \frac{\partial^2 g}{\partial y_1^i \partial y_2^j} \right) = D \left( \frac{1}{2r_1r_2} + \frac{1}{2r_1r_{12}} + \frac{1}{2r_2r_{12}} \right). \tag{3.10}
\]
Similarly, the transverse–traceless velocity-dependent terms, $\left[ \frac{4Gm_1}{c^4r_1} v_i^j v_1^j \right]^{TT}$ (and $1 \leftrightarrow 2$), in \((3.7)\) are given by
\[
\left[ \frac{4Gm_1}{c^4r_1} v_i^{<j} v_1^{j>} \right]^{TT} = \frac{Gm_1}{c^4r_1} \left[ \frac{1}{2} v_1^{(i} v_1^{j)} + \delta_{ij} \left( -\frac{5}{4} (n_1 v_1)^2 + \frac{1}{4} v_1^2 \right) + 3(n_1 v_1) n_1^{(i} v_1^{j)} + n_i^{ij} \left( \frac{3}{4} (n_1 v_1)^2 - \frac{5}{4} v_1^2 \right) \right], \tag{3.11}
\]
and $1 \leftrightarrow 2$, where $1 \leftrightarrow 2$ denotes the exchange of particle labels 1 and 2. In more detail, we have chosen in \((3.7)\) to fix the spatial coordinates, $x^i$, of the conformal 3-metric $\tilde{\gamma}_{ij}^{Dirac}$ on each hypersurface, $\Sigma_r$, in the generalized Dirac gauge, as introduced

\(^{20}\)This may be trivially seen by applying the transverse–traceless projection tensor, $^{TT} \delta_{ij}^{kl}$, given by \cite{68},
\[
^{TT} \delta_{ij}^{kl} = \delta_{ik} \delta_{jl} - \delta_{ij} \delta_{kl} \Delta^{-1} - \delta_{ij} \frac{1}{2} \delta_{kl} \Delta^{-1} + \frac{1}{2} \delta_{ik} \Delta^{-1} \delta_{jl}^{-1} + \frac{1}{2} \delta_{kl} \Delta^{-1} \delta_{ij}^{-1} - \frac{1}{2} \delta_{ij} \Delta^{-1} \delta_{kl}^{-1} \tag{3.6}
\]
on the symmetric-tracefree conformal 3-metric, $\tilde{\gamma}_{ij}$ \cite{81}.\]
The covariant generalized Dirac gauge is defined there as,

\[ D_j \left[ \left( \frac{\gamma}{f} \right)^{1/3} \gamma^{ij}_{\text{Dirac}} \right] = 0, \quad (3.12) \]

where \( f \) and \( D \) denote, respectively the determinant and the unique covariant derivative with respect to a flat metric, \( f_{ij} \) (in an arbitrary coordinate system). Equivalently, \( (3.12) \) may be expressed in terms of the conformal metric as \( \frac{\partial}{\partial x_j} \tilde{\gamma}^{ij}_{\text{Dirac}} = 0 \), where the flat metric \( f^{ij} \equiv \delta^{ij} \) assumes Minkowski coordinates.

Finally, from \( (3.8) \) and \( (3.11) \), the explicit form of \( (3.7) \) is given as,

\[
\tilde{\gamma}^{ij}_{\text{Dirac}} - \delta_{ij} = \frac{G^2 m_1 m_2}{c^4} \left[ \delta^{ij} \left( -\frac{5r_1}{8r_1^3} - \frac{15r_1^2}{8r_1^3 r_2} + \frac{5r_1^4}{8r_1^3 r_2^2} + \frac{1}{(r_1 + r_2 + r_1)^2} \right) 
+ \frac{r_1}{r_1^2} \right]
+ \frac{1}{r_2} \frac{\delta^{ij} \left( \frac{1}{r_1^2} + \frac{11}{8r_1^3 r_2} - \frac{2r_1^2}{2r_1^2 r_2} - \frac{1}{r_1^2} \left( \frac{7}{r_1^2} + \frac{7}{r_1^2} \right) \right)
+ n_i n_i^j \left( \frac{r_1}{8r_1^3} + \frac{11}{8r_1^3 r_2} - \frac{7}{8r_1^3 r_2} + \frac{7}{(r_1 + r_2 + r_1)^2} - \frac{7}{(r_1 + r_2 + r_1)^2} \right)
+ n_i n_i^j \left( \frac{2r_1^2}{2r_1^2 r_2} + \frac{1}{r_1^2} \left( \frac{7}{r_1^2} + \frac{7}{r_1^2} \right) \right)
+ \left( 4 \frac{r_1}{r_1^2} \right) \right]
+ Gm_1 c^3 \frac{v_i v_i^j}{2} + \delta^{ij} \left( -\frac{5(n_1 v_1)^2}{4} + \frac{v_1^2}{4} \right) + 3(n_1 v_1) n_i v_i^j
+ n_i n_i^j \left( \frac{3(n_1 v_1)^2}{4} - \frac{5v_1^2}{4} \right) \right) + 1 \leftrightarrow 2. \quad (3.13)\]

2. Extrinsic Curvature: \( \tilde{A}^{ij}_{\text{TT}} \) and \( K \)

The conformal symmetric transverse-tracefree tensor component of the extrinsic curvature, \( \tilde{A}^{ij}_{\text{TT}} \), is given by,

\[ \tilde{A}^{ij}_{\text{TT}} = 0, \quad (3.14) \]

for both possible values of \( K \): maximal hypersurface \( K = 0 \) and the post-Newtonian mean curvature \( K^{2\text{PN}} \) derived at 2PN using results in \( [56] \) and given by,

\[ K^{2\text{PN}} = \frac{Gm_1(n_1 v_1)}{c^3 r_1^2} + \frac{Gm_2(n_2 v_2)}{c^3 r_2^2} + \mathcal{O} \left( \frac{1}{c^5} \right). \quad (3.15) \]

The choice of \( \tilde{A}^{ij}_{\text{TT}} = 0 \) and \( K = 0 \) are in agreement at 2PN order with their counterparts in the standard Bowen-York solution, given in \( [27] \). Maximal slicing is considered advantageous.
primarily due to its ‘singularity avoiding’ feature during evolution; the slicing causes the lapse, \( N \), to collapse to zero in the region where a physical singularity exists; see \[69\] for a general discussion.

3. **Weight function: \( \tilde{\sigma} \)**

As is mentioned in Section II D, we consider two specific instances; a) \( \sigma = 2N \) and \( \tilde{\sigma} = 2\tilde{N} \) and, b) \( \tilde{\sigma} = 1 \).

(a) \( \sigma = 2N \) and \( \tilde{\sigma} = 2\tilde{N} \)

This concerns the class of solutions where the EC and CTS decompositions are seen to be equivalent. Depending on the choice in mean curvature, either \( K = 0 \) or \( K = K^{2\text{PN}} \), and whether the conformal 3-metric, \( \tilde{\gamma}_{ij} \), is specified in symmetric trace-free form or in Dirac coordinates (following the relationship \( N = \Psi^6\tilde{N} \)), the conformal weight function based on 2PN results, \( \tilde{\sigma}^{2\text{PN}} \), can take four different forms. These are:

i) For a maximal hypersurface \( K = 0 \), \( \tilde{\sigma}|_{K=0} \) is given as,

\[
\tilde{\sigma}^{\text{STT}}|_{K=0} - 2 \equiv 2\tilde{N}^{\text{STT}}|_{K=0} - 2 = -\frac{8Gm_1}{c^2r_1} + \frac{1}{c^4} \left[ \frac{Gm_1}{r_1} [3(n_1v_1)^2 - 7v_1^2] + \frac{35G^2m_1^2}{2c^4r_1^2} \right]
\]

\[
+ G^2m_1m_2 \left( \frac{18}{r_1r_2} + \frac{10}{r_{12}r_2} \right) + 1 \leftrightarrow 2, \quad (3.16)
\]

in a symmetric trace-free coordinate system.

ii) Similarly, in Dirac coordinates,

\[
\tilde{\sigma}^{\text{Dirac}}|_{K=0} - 2 \equiv 2\tilde{N}^{\text{Dirac}}|_{K=0} - 2 = -\frac{8Gm_1}{c^2r_1} + \frac{1}{c^4} \left[ -\frac{6Gm_1}{r_1} v_1^2 + \frac{35G^2m_1^2}{2c^4r_1^2} \right]
\]

\[
+ G^2m_1m_2 \left( \frac{35}{2r_1r_2} + \frac{5}{r_{12}r_2} \right) + 1 \leftrightarrow 2. \quad (3.17)
\]

iii) For the 2PN derived mean curvature \( K^{2\text{PN}} \), \( \tilde{\sigma}|_{K^{2\text{PN}}} \) is given as,

\[
\tilde{\sigma}^{\text{STT}}|_{K^{2\text{PN}}} - 2 \equiv 2\tilde{N}^{\text{STT}}|_{K^{2\text{PN}}} - 2 = -\frac{8Gm_1}{c^2r_1} + \frac{1}{c^4} \left[ \frac{Gm_1}{r_1} [4(n_1v_1)^2 - 8v_1^2] + \frac{35G^2m_1^2}{2c^4r_1^2} \right]
\]

\[
+ G^2m_1m_2 \left( \frac{18}{r_1r_2} + \frac{21}{2r_{12}r_2} + \frac{r_1}{2r_{12}^2} - \frac{r_1^2}{2r_{12}r_2^2} \right) + 1 \leftrightarrow 2,
\]

in the symmetric trace-free coordinate system.
iv) Similarly, in Dirac coordinates,

\[ \tilde{\sigma}_{\text{Dirac}}|_{K^{2\text{PN}}} - 2 \equiv 2\tilde{N}_{\text{Dirac}}|_{K^{2\text{PN}}} - 2 = -\frac{8Gm_1}{c^2r_1} + \frac{1}{c^4} \left[ \frac{Gm_1}{r_1} \left[ (n_1v_1)^2 - 7v_1^2 \right] + \frac{35G^2m_1^2}{2c^4r_1^2} \right] \\
+ G^2m_1m_2 \left( \frac{39}{2r_1r_2} + \frac{11}{2r_1r_2} + \frac{r_1}{2r_{12}} - \frac{r_1^2}{2r_{12}^2} \right) \\
+ 1 \leftrightarrow 2. \]

(b) \( \tilde{\sigma}^{\text{CTT}} \) in the CTT decomposition

In this case, the conformal weight function \( \tilde{\sigma}^{\text{CTT}} = 1 \).

B. CTS Decomposition

We now present each of the components in the free data (\( \tilde{\gamma}_{ij}, \tilde{u}_{ij}, K, \tilde{N} \) or \( \partial_t K \)).

1. Conformal metric: \( \tilde{\gamma}_{ij} \)

Due to the identical nature of the conformal decompositions of the 3-metric \( \gamma_{ij} \), the post-Newtonian motivated conformal metric in symmetric-tracefree form, \( \tilde{\gamma}_{ij} \), and in Dirac coordinates, \( \tilde{\gamma}_{ij}^{\text{Dirac}} \), are given by (3.1) and (3.7) respectively.

2. Time derivative of the conformal metric, \( \tilde{u}_{ij} \), and mean curvature \( K \)

Following definition (2.15) and using either \( \gamma_{ij} \) (3.1) or \( \tilde{\gamma}_{ij} \) (3.7), we propose that the post-Newtonian time derivative of the conformal metric, \( \tilde{u}_{ij} \), adopts the form,

\[ \tilde{u}^{ij} = 0, \quad (3.18) \]

at 2PN for both a maximal hypersurface, \( K = 0 \), and the 2PN derived mean curvature \( K^{2\text{PN}} \), given by (3.15). The particular choice in \( \tilde{u}_{ij} = 0 \) and \( K = 0 \) are in agreement with quasi-stationary initial conditions\(^{21} 28, 29, 38, 39 \).

\(^{21}\) Note that helical symmetry is exact with respect to Newtonian and 2PN gravity.
3. Conformal Lapse $\tilde{N}$, or time derivative of mean curvature, $\partial_t K$

As discussed in Section II C, we give both the conformal lapse, $\tilde{N}$, and the time derivative of mean curvature, $\partial_t K$, depending on whether the simple, or the extended, CTS system of constraint equations is to be used.

(a) Conformal Lapse $\tilde{N}$

Thanks to the choice in both mean curvature, $K = 0$ or $K^{2\text{PN}}$, and the preferred spatial coordinate system of $\tilde{\gamma}_{ij}$ or $\tilde{\gamma}_{ij}^{\text{Dirac}}$, there are four different possibilities for the 2PN based conformal lapse, $\tilde{N}$. These are:

i) For a maximal hypersurface $K = 0$, $\tilde{N}|_{K=0}$ is given as,

$$\tilde{N}^{\text{STT}}|_{K=0} - 1 = -\frac{4Gm_1}{c^2 r_1} + \frac{1}{c^4} \left[ \frac{Gm_1}{r_1} \left( \frac{3}{2} (n_1 v_1)^2 - \frac{7v_1^2}{2} \right) + \frac{35G^2m_1^2}{4c^4 r_1^2} + G^2 m_1 m_2 \left( \frac{9}{r_1 r_2} + \frac{5}{r_2 r_1} \right) \right] + 1 \leftrightarrow 2, \quad (3.19)$$

in the symmetric trace-free coordinate system.

ii) Similarly, in Dirac coordinates,

$$\tilde{N}^{\text{Dirac}}|_{K=0} - 1 = -\frac{4Gm_1}{c^2 r_1} + \frac{1}{c^4} \left[ -\frac{3Gm_1}{r_1} v_1^2 + \frac{35G^2m_1^2}{4c^4 r_1^2} + G^2 m_1 m_2 \left( \frac{35}{4r_1 r_2} + \frac{5}{2r_1 r_2} \right) \right] + 1 \leftrightarrow 2. \quad (3.20)$$

iii) For the 2PN derived mean curvature $K^{2\text{PN}}$, $\tilde{N}|_{K^{2\text{PN}}}$ is given as,

$$\tilde{N}^{\text{STT}}|_{K^{2\text{PN}}} - 1 = -\frac{4Gm_1}{c^2 r_1} + \frac{1}{c^4} \left[ \frac{Gm_1}{r_1} \left[ 2(n_1 v_1)^2 - 4v_1^2 \right] + \frac{35G^2m_1^2}{4c^4 r_1^2} + G^2 m_1 m_2 \left( \frac{9}{r_1 r_2} + \frac{21}{4r_1 r_2} + \frac{r_1}{4r_1^2} - \frac{r_2^2}{4r_1^2} \right) \right] + 1 \leftrightarrow 2, \quad (3.21)$$

in the symmetric trace-free coordinate system.

iv) Similarly, in Dirac coordinates,

$$\tilde{N}^{\text{Dirac}}|_{K^{2\text{PN}}} - 1 = -\frac{4Gm_1}{c^2 r_1} + \frac{1}{c^4} \left[ \frac{Gm_1}{r_1} \left( \frac{(n_1 v_1)^2}{2} - \frac{7v_1^2}{2} \right) + \frac{35G^2m_1^2}{4c^4 r_1^2} + G^2 m_1 m_2 \left( \frac{39}{4r_1 r_2} + \frac{11}{4r_1^2} + \frac{r_1}{4r_1^2} - \frac{r_2^2}{4r_1^2} \right) \right] + 1 \leftrightarrow 2. \quad (3.22)$$
(b) **Time derivative of mean curvature, $\partial_t K$**

Since there exist two alternative slicing possibilities for our PN free data, $K = 0$ or $K \equiv K^{2\text{PN}}$, their time derivatives are given respectively by: i) $\partial_t K = 0$, or ii) 

$$
\partial_t K^{2\text{PN}} = \frac{G m_1}{c^4 r_1^3} (3(n_1 v_1)^2 - v_1^2) + \frac{G^2 m_1 m_2}{c^4 r_{12}} \left( \frac{1}{2r_1^2 r_{12}} + \frac{1}{2r_1^3} - \frac{r_1^2}{2r_{12}^2 r_2^2} \right) + 1 \leftrightarrow 2 + \mathcal{O} \left( \frac{1}{c^5} \right),
$$

(3.23)

## IV. PROOF OF EQUIVALENCE WITH POST-NEWTONIAN RESULTS

This section presents our reasoning behind the choice of free data discussed in Section III and, in particular, their full agreement with post-Newtonian results at 2PN order. Note that the free data are also chosen such that they satisfy the constraints, albeit approximately. In illustrating this agreement, we state first in Section IV A our central result exhibiting the “near zone” behavior of the proposed solution and outline then its derivation in Section IV B by considering the form of the proposed PN-derived conformal 3-metrics, $\tilde{\gamma}_{ij}$ and $\tilde{\gamma}_{ij}^{\text{Dirac}}$. In addition, motivations for the specific form of our PN free data are given in Section IV C by considering the lowest order perturbation of the Bowen-York solution. This allows us to investigate both the global structure and near-zone solution of our proposed PN based solution. Finally, in Section IV D we show that our results imply that the physical extrinsic curvature from the standard Bowen-York solution, $K_{ij}^{\text{B-Y}}$, and post-Newtonian derived counterpart, $K_{ij}^{2\text{PN}}$, are physically equivalent.

### A. Statement of Equivalence

The statement of equivalence presented below is a generalization of Theorem 1 in [1] for stationary black holes to moving black holes with $\mathbf{v}_1, \mathbf{v}_2 \neq 0$.

The conformal metrics, $\tilde{\gamma}_{ij}$ and $\tilde{\gamma}_{ij}^{\text{Dirac}}$, are chosen in such a way that a post-Newtonian expansion (when $c \to \infty$) of their corresponding physical metrics, $\gamma_{ij} = \Psi^4 \tilde{\gamma}_{ij}$ and $\gamma_{ij}^{\text{Dirac}} = (\Psi^{\text{Dirac}})^4 \tilde{\gamma}_{ij}^{\text{Dirac}}$, are physically equivalent to the standard post-Newtonian spatial metric in harmonic coordinates at 2PN order, that is, they differ only by a change of coordinates. This can be stated as,

$$
\gamma_{ij} = g_{ij}^{2\text{PN}} + \partial_i \xi_j + \partial_j \xi_i + \mathcal{O} \left( \frac{1}{c^5} \right),
$$

(4.1)

\[ \text{23} \]
A similar statement applies to Dirac coordinates. In other words,

$$\gamma_{ij}^{\text{Dirac}} = g_{ij}^{2\text{PN}} + \partial_i \xi_{j}^{\text{Dirac}} + \partial_j \xi_{i}^{\text{Dirac}} + \mathcal{O}\left(\frac{1}{c^5}\right).$$

In (4.1) and (4.2), \(g_{ij}^{2\text{PN}}\) represents the spatial metric in harmonic coordinates truncated at 2PN order. The remainder \(\mathcal{O}\left(\frac{1}{c^5}\right)\) accounts for neglected 2.5PN and higher-order terms. The change in coordinates is specified by the unique spatial gauge transformation, \(\xi^i\) or \(\xi_{i}^{\text{Dirac}}\), depending on the preferred coordinate system.

Additionally, our PN data obeys the following relationships for either maximal slicing, \(K = 0\),

$$\gamma_{0i} = g_{0i}^{2\text{PN}} + \partial_0 \xi_{i} + \partial_i \xi_0 + \mathcal{O}\left(\frac{1}{c^5}\right),$$

$$\gamma_{00} = g_{00}^{2\text{PN}} + 2 \partial_0 \xi_0 + \mathcal{O}\left(\frac{1}{c^5}\right),$$

or, mean curvature \(K_{2\text{PN}}\),

$$\gamma_{0i}^\prime = g_{0i}^{2\text{PN}} + \partial_0 \xi_{i}^\prime + \partial_i \xi_0^\prime + \mathcal{O}\left(\frac{1}{c^5}\right),$$

$$\gamma_{00}^\prime = g_{00}^{2\text{PN}} + 2 \partial_0 \xi_0^\prime + \mathcal{O}\left(\frac{1}{c^5}\right),$$

where \(\xi_i = \xi_i + \mathcal{O}(1/c^5)\) and \(g_{00}^{2\text{PN}}\) and \(g_{0i}^{2\text{PN}}\) represent the 00th and 0i component of the full spacetime metric in harmonic coordinates.

The vector, \(\xi^\mu\), which is determined by (4.1)–(4.6), represents unique infinitesimal gauge transformation (i.e. \(x^\mu \rightarrow x'^\mu = x^\mu + \xi^\mu(x^\nu)\), where \(\{x^\mu\}\) and \(\{x'^\mu\}\) are two general coordinate systems) at 2PN order and is explicitly given by the following components,

$$\xi_0 = \frac{Gm_1}{2c^3}(n_1 v_1) + \frac{Gm_2}{2c^3}(n_2 v_2) + \mathcal{O}\left(\frac{1}{c^4}\right),$$

$$\xi_0^\prime = 0 + \mathcal{O}\left(\frac{1}{c^5}\right),$$

for either mean curvature \(K = 0\) or \(K_{2\text{PN}}\) respectively,

$$\xi_i = \frac{G^2 m_1^2}{4c^4} \partial_i \ln r_1 + \frac{G^2 m_2^2}{4c^4} \partial_i \ln r_2 + \mathcal{O}\left(\frac{1}{c^5}\right),$$

for the symmetric trace-free coordinate system and, similarly, in Dirac coordinates,

$$\xi_{i}^{\text{Dirac}} = \frac{G^2 m_1^2}{4c^4} \partial_i \ln r_1 - \frac{7G^2 m_1 m_2}{2c^4} \frac{n_1}{(r_1 + r_2 + r_12^2)} + \frac{3G^2 m_1 m_2}{8c^4} \partial_i \left( \frac{r_1 + r_2}{r_12} \right)$$

$$- \frac{G^2 m_1 m_2}{c^4} \partial_i \left( \frac{r_2 - r_1}{r_12} \right) - \frac{G^2 m_1 m_2}{4c^4} \partial_i D \left( \frac{r_3^1 + r_3^2}{r_12} \right) - \frac{2Gm_1}{c^4} \partial_k \left( v_{k}^{(i)} v_{k}^{(l)} r_1 \right)$$

$$+ \frac{Gm_1}{2c^4} \partial_{ikl} \left( v_{1}^{(k)} v_{1}^{(l)} r_1^3 \right) + \frac{Gm_1}{2c^4} \partial_i (v_1^2 r_1) + 1 \leftrightarrow 2 + \mathcal{O}\left(\frac{1}{c^5}\right).$$

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B. Relationship between the conformal metrics, $\tilde{\gamma}_{ij}$ and $\tilde{\gamma}^{\text{Dirac}}_{ij}$, and the post-Newtonian metric

In order to demonstrate results (4.1) and (4.2), let us consider initially a post-Newtonian iteration of the Hamiltonian constraint, (2.14) and (2.18), for proposed conformal metric in symmetric-trace-free form, $\tilde{\gamma}_{ij}$, at 2PN order,

$$\Delta \Psi = -\frac{G^2 m_1 m_2}{c^4} \partial_{ij} \left( <i g_{j}> \right) + \frac{G m_1}{2 c^4 r_1^3} (n_1 v_1) + \frac{G m_2}{2 c^4 r_2^3} (n_2 v_2) + \mathcal{O} \left( \frac{1}{c^5} \right), \quad (4.11)$$

where we note the absence of any contributing terms from the extrinsic curvature, $K_{ij}$. As Section IV D shows, this is unsurprising considering that the lowest order term in the extrinsic curvature, $K_{ij}$, appears at $\mathcal{O} \left( \frac{1}{c^3} \right)$. Therefore, the quadratic terms of the conformal symmetric transverse-trace-free tensor $\tilde{A}_{ij}^{TT}$, and mean curvature, $K$, occur at order $\mathcal{O} \left( \frac{1}{c^6} \right)$ in (2.14) and (2.18). The most general solution to (4.11), in the full distributional sense, for the conformal factor, $\Psi$, is given by,

$$\Psi = \psi - \frac{G^2 m_1 m_2}{2 c^4} \frac{D}{g} \left( \frac{g}{3} + \frac{r_1 + r_2}{2 r_{12}} \right) - \frac{G m_1}{12 c^4 r_1} \left( 3 (n_1 v_1)^2 - v_1^2 \right) - \frac{G m_2}{12 c^4 r_2} \left( 3 (n_2 v_2)^2 - v_2^2 \right) + \mathcal{O} \left( \frac{1}{c^5} \right), \quad (4.12)$$

$\psi$ being the solution of the homogenous equation, $\Delta \psi = 0$. This result, when instantiated with $v_1 = v_2 = 0$, is consistent with the time-symmetric result of [1], given there by Eqns. (2.6) and (2.7). The explicit form of $\psi$ is then obtained by comparing (4.12) with the post-Newtonian spatial metric, $g_{ij}^{\text{2PN}}$ (i.e. Eqn. (7.2) in [56]) in the form,

$$\psi = 1 + \frac{G m_1}{2 c^2 r_1} \left( 1 - \frac{G m_2}{2 c^2 r_{12}} + \frac{v_1^2}{2 c^2} \right) + \frac{G m_2}{2 c^2 r_2} \left( 1 - \frac{G m_1}{2 c^2 r_{12}} + \frac{v_2^2}{2 c^2} \right) + \mathcal{O} \left( \frac{1}{c^5} \right). \quad (4.13)$$

Since further ‘homogeneous’ terms $\sim 1/r_1$ and $\sim 1/r_2$ can be added to $\Psi$, without affecting (4.11), for consistency, we specify that $\Psi$ must satisfy (4.11) in a strict distributional sense; see Section III A in [1]. Therefore, we do not allow the addition of such terms, here and henceforth, to our solutions for Poisson-type equations.

Interestingly, by re-expressing $\psi$, (4.13), in terms of ‘Brill-Lindquist-like’ constants, $\alpha_1$ and $\alpha_2$,

$$\psi \equiv 1 + \frac{\alpha_1}{r_1} + \frac{\alpha_2}{r_2}, \quad (4.14)$$

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where $\alpha_1$ and $\alpha_2$ are determined to the relative 2PN accuracy from (4.13) as,

\[
\alpha_1 = \frac{Gm_1}{2c^2} \left( 1 - \frac{Gm_2}{2c^2r_{12}} + \frac{v_1^2}{2c^2} + \mathcal{O} \left( \frac{1}{c^3} \right) \right) \quad \text{and} \quad 1 \leftrightarrow 2, \quad (4.15)
\]

we recover the original Brill-Lindquist conformal factor, $\psi_{\text{BL}}$, for the time-symmetric instance $v_1 = v_2 = 0$ at 2PN order\(^{22}\).

In contrast, when following a similar procedure for Dirac coordinates, we find that the conformal factor $\Psi^{\text{Dirac}}$ is equivalent to the term $\psi$, (4.13), i.e.

\[
\Psi^{\text{Dirac}} \equiv \psi = 1 + \alpha_1 \frac{r_1}{r_2} + \alpha_2 \frac{r_2}{r_1} = 1 + \frac{Gm_1}{2c^2r_1} \left( 1 - \frac{Gm_2}{2c^2r_{12}} + \frac{v_1^2}{2c^2} \right) + \frac{Gm_2}{2c^2r_2} \left( 1 - \frac{Gm_1}{2c^2r_{12}} + \frac{v_2^2}{2c^2} \right) + \mathcal{O} \left( \frac{1}{c^5} \right). \quad (4.17)
\]

Therefore, the deviation of our post-Newtonian motivated solution from the conformally flat solution in the Dirac gauge manifests itself solely as a perturbation in the conformal metric, $\tilde{\gamma}^{\text{Dirac}}_{ij}$, (3.7), and not to the ‘Brill-Lindquist’-like conformal factor, $\psi$ (4.13), at the 2PN order.

### C. Perturbation of a general global conformally–flat solution

This section considers the lowest order perturbation of the standard conformally-flat Bowen-York solution. It gives an insight into the specific form of the conformal 3 metric, $\tilde{\gamma}_{ij}$. Note that we only consider the symmetric trace-free form of the proposed conformal metric, $\tilde{\gamma}_{ij}$ (3.1). This is because, as discussed in Section IV B, the PN based conformal metric in Dirac coordinates, $\tilde{\gamma}^{\text{Dirac}}_{ij}$ (3.7), incorporates fully the characteristics of the 2PN metric itself and does not incur a perturbative change to the Brill-Lindquist-like conformal factor, $\psi$ (4.13).

\[^{22}\] $\psi_{\text{BL}}$ is given here for completeness as,

\[
\psi^{B-L} = 1 + \frac{\alpha^{B-L}_1}{r_1} + \frac{\alpha^{B-L}_2}{r_2} = 1 + \frac{Gm_1}{2c^2r_1} \left( 1 - \frac{Gm_2}{2c^2r_{12}} \right) + \frac{Gm_2}{2c^2r_2} \left( 1 - \frac{Gm_1}{2c^2r_{12}} \right) + \mathcal{O} \left( \frac{1}{c^5} \right). \quad (4.16)
\]
Let us introduce formally a metric perturbation, $h_{ij}$, to the conformal metric $\tilde{\gamma}_{ij}$, where we interpret the proposed 2PN motivated conformal metric (3.1) as a perturbation to the Bowen-York solution, i.e.,

$$\tilde{\gamma}_{ij} = \delta_{ij} + h_{ij},$$

(4.18)

where $h = h_{ii} = 0$ and $h_{ij}$ is explicitly given from (3.1) as,

$$h_{ij} = -\frac{8G^2 m_1 m_2}{c^4} \frac{\partial^2 g}{\partial y^i_1 \partial y^j_2} + \frac{4Gm_1}{c^4 r_1} v^i_1 v^j_1 + \frac{4Gm_2}{c^4 r_2} v^i_2 v^j_2.$$

(4.19)

Consequently, the conformal factor, $\Psi$, must include a perturbation, $\kappa$, to the “Brill-Lindquist-like” conformal factor, $\psi$, such that,

$$\Psi = \psi + \kappa,$$

(4.20)

where $\psi$ is given by (4.13) and its structure is chosen to resemble as closely as possible the form of the time-symmetric, Brill-Lindquist conformal factor, $\psi_{B-L}$ (4.16).

We then assume that $\kappa$, the perturbation in the conformal factor, and $\tilde{K}_{ij}$, the full conformal extrinsic curvature, admit power-like expansions of the type,

$$\kappa = \sum_{n=2}^{+\infty} \left( \frac{1}{c^{2n}} \right) \kappa_{(n/2)},$$

(4.21)

$$\tilde{K}_{ij} = \sum_{n=1}^{+\infty} \left( \frac{1}{c^{2n+1}} \right) \tilde{K}_{(n+1/2)ij}.$$ 

(4.22)

Subtle considerations determine the form of the above expansions. Notably, we introduce formally the expansions to investigate perturbations to the Bowen-York solution. They do not, as they might otherwise misleadingly suggest, represent post-Newtonian expansions in the general sense. Instead, the parameter $c$ tracks the order of the perturbation to the Bowen-York solution. Consequently, the lowest order of the perturbation metric for a non-zero extrinsic curvature, $h_{ij}|_{K_{ij}\neq0}$, is to be of $O(1/c^4)$. In this light, it is therefore more appropriate to regard the resulting perturbation equations (at low order) as successive integer approximations in the perturbative metric, $h_{ij}$, of the conformally-flat solution. Note that our definition (4.22) determines the zeroth order term in $\tilde{K}_{ij}$ (i.e. $\tilde{K}_{(2)ij}$) to be of $O(1/c^3)$, which is dimensionally consistent with both $K_{ij}^{2PN}$ and $\tilde{K}_{ij}^{B-Y}$, as given later by (4.31) and (4.37) respectively.
1. Analytic closed form of the linearized solution

By considering the formal perturbation, as defined by (4.21) and (4.22), of constraint (2.9) together with (2.13) and (2.17), we arrive at the linearized perturbation of the Hamiltonian constraint,

\[ \tilde{\Delta} \kappa(1) = h^{ij} \partial_{ij} \Psi + \partial_i h^k_i \partial_k \Psi + \frac{1}{8} \Psi \partial_{ij} h_{ij}. \]  

(4.23)

The above is identical in form to its counterpart in the case of a linear perturbation to the time-symmetric Brill-Lindquist constraints, given by Eqn. (3.7) in [1]. In contrast, the linear–order terms in (4.23) in both the perturbation metric, \( h_{ij} \) (4.19), and Brill-Lindquist-like conformal factor, \( \psi \) (4.13), include terms due to the velocity of the black holes. On the other hand, we may identify the time-independent parts in \( h_{ij} \) and \( \psi \), (4.19) and (4.13) respectively, and refer to the results given in Section III B in [1] for solving the time-symmetric components in (4.23). Substitution of (4.19) and (4.20) into (4.23), allows us to determine the exact solution for \( \kappa(1) \),

\[ \kappa(1) = -G^2 m_1 m_2 D \left[ \frac{g}{6} + \frac{r_1 + r_2}{4r_{12}} \right] - \frac{Gm_1}{r_1} \left[ \frac{(n_1 v_1)^2}{4} - \frac{v_1^2}{12} \right] - \frac{Gm_2}{r_2} \left[ \frac{(n_2 v_2)^2}{4} - \frac{v_2^2}{12} \right] \]

\[ + \alpha_1 \left\{ -G^2 m_1 m_2 \left[ 4H_1 + \frac{K_1}{4} - \frac{1}{4} \left( \frac{1}{r_2} \ln \left[ \frac{r_1}{r_{12}} \right] \right) \right] + \frac{9}{4} \left( \ln \frac{r_1}{r_{12}} \right) + \frac{2Dg}{r_1} \right\} + \alpha_2 \{ 1 \leftrightarrow 2 \} \]

\[ = -G^2 m_1 m_2 D \left[ \frac{g}{6} + \frac{r_1 + r_2}{4r_{12}} \right] - \frac{Gm_1}{r_1} \left[ \frac{(n_1 v_1)^2}{4} - \frac{v_1^2}{12} \right] - \frac{Gm_2}{r_2} \left[ \frac{(n_2 v_2)^2}{4} - \frac{v_2^2}{12} \right] \]

\[ + \alpha_1 \left\{ -G^2 m_1 m_2 \left[ 4\Delta_1 \left[ \frac{g}{r_{12}} + D \left( \frac{r_1 + r_{12}}{2g} \right) \right] - 4D \left( \ln \frac{r_{12}}{r_1} \right) - \frac{15}{4} D \left( \ln \frac{r_1}{r_{12}} \right) \right] \right\} + \alpha_2 \{ 1 \leftrightarrow 2 \} \]

\[ = -G^2 m_1 m_2 \left[ \frac{g}{6} + \frac{r_1 + r_2}{4r_{12}} \right] - \frac{Gm_1}{r_1} \left[ \frac{(n_1 v_1)^2}{4} - \frac{v_1^2}{12} \right] - \frac{Gm_2}{r_2} \left[ \frac{(n_2 v_2)^2}{4} - \frac{v_2^2}{12} \right] \]

\[ + \alpha_1 \left\{ -G^2 m_1 m_2 \left[ 4\Delta_1 \left[ \frac{g}{r_{12}} + D \left( \frac{r_1 + r_{12}}{2g} \right) \right] - 4D \left( \ln \frac{r_{12}}{r_1} \right) - \frac{15}{4} D \left( \ln \frac{r_1}{r_{12}} \right) \right] \right\} + \alpha_2 \{ 1 \leftrightarrow 2 \}, \]

(4.25)

where \( \Delta_1 = \frac{\partial^2}{\partial y_1^2} \) and \( \Delta_2 = \frac{\partial^2}{\partial y_2^2} \) denote the Laplacians with respect to the source positions \( y_1 \) and \( y_2 \) respectively, and \( D = \frac{\partial^2}{\partial y_1^2 \partial y_2^2} \) as before. As pointed out earlier, the results (3.8) and (3.11) in [1] may be used in the above. The expression for \( \kappa(1) \) (4.25) is valid in the full
distributional sense, i.e. the addition of an arbitrary number of ‘homogeneous’ terms \( \sim 1/r_1 \)
and \( \sim 1/r_2 \) is not permitted, as mentioned earlier, when solving the Poisson-type equation for \( \kappa_{(1)} \). Note that \( \kappa_{(1)} \) also tends to zero at spatial infinity (i.e. when \( r \equiv |x| \to +\infty \)). Consistent with Eqns. (3.8) and (3.11) in [1], only terms in the first line of (4.24) and (4.25) contribute at the 2PN order in the conformal factor, \( \Psi \). The additional terms, which are proportional to 1PN constants, \( \alpha_1 \) or \( \alpha_2 \), appear only at the 3PN order. Indeed, (4.25) reflects characteristic 3PN features, despite imposing only the initial isometric relationship with a 2PN expansion, (4.1). In particular, the intermediate expression, (4.24), contains the special Poisson-like solutions \( H_1 \) and \( K_1 \), which appear in the 3PN spatial metric, given by Eqn. (111) in [67]. For completeness, we include here the functions, \( H_1 \) and \( K_1 \), satisfying the following Poisson-like equations,

\[
\Delta H_1 = 2 \, g_{ij} \partial_{ij} \left( \frac{1}{r_1} \right),
\]

\[
\Delta K_1 = 2D^2 \left( \frac{\ln r_1}{r_2} \right),
\]

and can be found as,

\[
H_1 = \Delta_1 \left[ \frac{g}{2r_{12}} + D \left( \frac{r_1 + r_12}{2} g \right) \right] - D \left( \frac{\ln r_{12}}{r_1} \right) - \frac{3}{2} D \left( \frac{\ln r_1}{r_{12}} \right) - \frac{r_2}{2r_1^2 r_{12}}
+ \frac{1}{2r_1^2 r_{12}} - \frac{1}{2r_1 r_{12}^2},
\]

\[
K_1 = D \left( \frac{1}{r_2} \ln \left[ \frac{r_1}{r_2} \right] \right) - \frac{1}{2r_1^2 r_2} + \frac{1}{2r_2 r_{12}^2} + \frac{r_2}{2r_1^2 r_{12}}.
\]

Finally, although (4.24) and (4.25) indicate 3PN characteristics, it is important to note that they do not represent complete expressions for \( \kappa_{(1)} \) at 3PN. Such an expression is only possible if we consider terms of 3PN order in \( h_{ij} \) (i.e. using 3PN results such as given in [67]), which we have not attempted here. Furthermore, in order to be strictly correct up to and including order \( \mathcal{O}(1/c^6) \), we should instead solve for \( \kappa_{(3/2)} \) by considering the 1.5 linear order equation to the conformally-flat Hamiltonian and momentum constraints, containing the first explicit appearance of the extrinsic curvature, \( K_{ij} \), in the hierarchy or perturbative equations:

\[
\tilde{\Delta} \kappa_{(3/2)} - h^{ij} \partial_{ij} \Psi - \partial_i h^k_i \partial_k \Psi - \frac{1}{8} \Psi \partial_{ij} h_{ij} - \frac{1}{12} \Psi^5 K_{[3/2]}^2 + \frac{1}{8} \Psi^5 \tilde{K}_{[3/2]ij} \tilde{K}_{[3/2]}^{ij} = 0,
\]

\[
23 \text{ These occur in the non-linear potential, } \hat{X}.
\]
\[ \nabla_j \left( \hat{K}^{ij}_{[3/2]} - \delta^{ij} K_{[3/2]} \right) = 0. \quad (4.31) \]

Such an investigation is beyond the scope of the current work.

Finally, the fully explicit form of \( \kappa_{(1)} \), obtained by expanding all the derivatives in the result (4.25), is given here for completeness as:

\[
\kappa_{(1)} = -G^2 m_1 m_2 \left[ \frac{1}{12r_1 r_2} + \frac{r_1 + r_2}{8r_1^3} + \frac{1}{24r_1} \left( \frac{1}{r_1} + \frac{1}{r_2} \right) - \frac{1}{24r_2^3} \left( \frac{r_2^2}{r_1} + \frac{r_1^2}{r_2} \right) \right] - Gm_1 \left[ \frac{(n_1 v_1)^2}{4r_1} - \frac{v_1^2}{12r_1} \right] - Gm_2 \left[ \frac{(n_2 v_2)^2}{4r_2} - \frac{v_2^2}{12r_2} \right] + \alpha_1 \left\{ -G^2 m_1 m_2 \left[ -\frac{2}{r_1^3} - \frac{13}{8r_1^3} \right] - \frac{1}{3r_1 r_1^2} - \frac{24r_1^3}{r_1^3} + \frac{4}{r_2^3} - \frac{8r_2^3}{r_1^3} + \frac{3}{8r_1 r_2^3} - \frac{1}{24r_1 r_2^3} + \frac{2r_2}{r_1^3} \right\] + Gm_2 \left[ \frac{(n_1 v_1)^2 - (n_2 v_2)^2}{2S^2} + \frac{4(n_1 v_1)(n_2 v_2)}{S^2} \right] - \frac{(n_2 v_2)^2}{2r_1 S} - \frac{(n_1 v_1)^2}{2r_2 S} + \frac{(n_1 v_1)^2}{2r_2 S} + \frac{4v_2^2}{r_1 S} + \frac{v_2^2}{2r_2 S} - \frac{2v_2^2}{3r_1 r_2} \right\} + \alpha_2 \{ 1 \leftrightarrow 2 \}. \quad (4.32) \]

where \( S = (r_1 + r_2 + r_1 r_2) \).

D. Choice of Extrinsic Curvature and Maximal Slicing

Despite their manifestly different forms, we show here that the physical extrinsic curvature of the conformally-flat Bowen-York solution, \( K_{ij}^{BY} \), and the extrinsic curvature derived from 2PN results, \( K_{ij}^{2PN} \), are physically equivalent to each other modulo the infinitesimal coordinate transformation specified by \( \xi^\mu \), as given by (4.7)–(4.10). In particular, we show the following relationship,

\[
K_{ij}^{BY} = K_{ij}^{2PN} + \partial_{ij} \xi_0 + \mathcal{O} \left( \frac{1}{c^4} \right), \quad (4.33)\]

where \( \xi_0 \) refers to the 0th (covariant) component of the gauge vector \( \xi^\mu \) and is specified by (4.7). The extrinsic curvature derived from post-Newtonian results \( K_{ij}^{2PN} \), at 2PN order is given by,

\[
K_{ij}^{2PN} = \frac{Gm_1}{c^3 r_1^2} \left( 4n_1(i v_{ij}) - \delta_{ij}(n_1 v_1) \right) + 1 \leftrightarrow 2 + \mathcal{O} \left( \frac{1}{c^4} \right), \quad (4.34)\]

30
On the other hand, the conformal Bowen-York extrinsic curvature, $\tilde{K}_{ij}^{\text{BY}}$, is given by,

$$
\tilde{K}_{ij}^{\text{BY}} = \frac{3Gm_1}{2c^3r_1^2} [2v_1(n_{1j}) - (n_1v_1)(\delta_{ij} - n_{1i}n_{1j})] + 1 \leftrightarrow 2. \quad (4.37)
$$

We hence denote the physical Bowen-York extrinsic curvature as $K_{ij}^{\text{BY}} = \Psi^2 \tilde{K}_{ij}^{\text{BY}}$, where $\Psi$ is given by (4.12) in symmetric tracefree form and by (4.17) in Dirac coordinates. Therefore, by considering terms up to $O(1/c^5)$, $K_{ij}^{\text{BY}} = \tilde{K}_{ij}^{\text{BY}} + O(1/c^5)$.

Note that, at first sight, the relationship (4.33) appears to contradict the standard transformation law of tensors. For completeness, we state the standard transformation law of tensors for $K_{ij}$ in the instance of an infinitesimal change of coordinates, $\{x^\mu\} \to \{x'^\mu\}$,

$$
\tilde{K}'_{\mu\nu} = \frac{\partial x^\sigma}{\partial x'^\mu} \frac{\partial x^\rho}{\partial x'^\nu} K_{\sigma\rho},
$$

such that the spatial components of the extrinsic curvature transform at linear order in $\xi^\mu$ are given by,

$$
K_{ij} = \tilde{K}'_{ij} + 2\partial_i(\xi_j) + O(\xi^2). \quad (4.38)
$$

If we relabel $K_{ij} \equiv K_{ij}^{2\text{PN}}$, the difference between (4.33) and (4.38) is immediately evident.

We stress, however, that despite this apparent contradiction, both equations are valid. The distinctions between the two 3–dimensional extrinsic curvatures, $K_{ij}^{\text{B–Y}}$ (which we relabel

\footnote{Strictly speaking, the Bowen–York conformal extrinsic curvature, $\tilde{K}_{ij}^{\text{fullB–Y}}$, is the solution to the constraints in the case of conformally flat (i.e. $\tilde{\gamma}_{ij} = \delta_{ij}$) vacuum spacetimes with a maximal hypersurface, $K = 0$, and is explicitly given by,

$$
\tilde{K}_{ij}^{\text{fullB–Y}} = \frac{3Gm_1}{2c^3r_1^2} [2v_1(n_{1j}) - (n_1v_1)(\delta_{ij} - n_{1i}n_{1j})]
\\quad + \frac{3Gm^2a}{2c^3r_1^4} [2v_1(n_{1j}) + (n_1v_1)(\delta_{ij} - n_{1i}n_{1j})] + 1 \leftrightarrow 2. \quad (4.35)
$$

where we consider only the linear momentum term (with no intrinsic angular momentum) of the original solution. The second term in (4.35) corresponds to its “inversion-symmetric term”; see \textsuperscript{27}. This complete solution (4.35) was chosen historically to generalize the two–sheeted topology of the Misner–Lindquist time–symmetric approach. As a result, the inversion–symmetric term satisfies the isometry condition for a field to exist on a two–sheeted manifold. The constant $a$ in (4.35) denotes the radius of the inversion sphere, or alternatively, the throat of the black hole after applying appropriate boundary conditions. Importantly, our approach does not concern itself directly with the topological nature of the two black holes. Therefore, we only refer to part of the Bowen-York solution for the most general topologies, $\tilde{K}_{ij}^{\text{BY}}$ (henceforth referred to as ‘Bowen-York’), where

$$
\tilde{K}_{ij}^{\text{BY}} = \frac{3Gm_1}{2c^3r_1^2} [2v_1(n_{1j}) - (n_1v_1)(\delta_{ij} - n_{1i}n_{1j})] + 1 \leftrightarrow 2. \quad (4.36)
$$

By general topologies, we include both the two-sheeted asymptotically flat universe Misner–Lindquist \textsuperscript{53} and three-sheeted Brill-Lindquist \textsuperscript{55} solutions.}
Specifically, the 3-extrinsic curvature, $\bar{K}'_{ij}$, given by \(4.33\) and \(4.38\) respectively, reveal the nature of the 3+1 foliation of the spacetime associated with a gauge transformation $^{25}$.

Let us now outline the proof of the relationship \(4.34\) between the two extrinsic curvatures, $K'_{ij}$ and $\bar{K}'_{\mu\nu}$. This can be understood by first considering the infinitesimal difference, $\delta n'_\nu$, between the time-like normal vectors, $\bar{n}'_\mu$ and $n'_\mu$,

$$\delta n'_\nu = \bar{n}'_\nu - n'_\nu, \quad (4.39)$$

where $\bar{n}'^\mu$ and $n'^\mu$ denote two distinct physical vectors in the coordinate system $\{x'^\mu\}$, which result from the transformation equations \(4.33\) and \(4.38\) respectively. From $n'^\mu \equiv -N\nabla^\mu t$ and using the standard tensor transformation law \(4.38\), it is possible to obtain explicit covariant and contravariant expressions for \(4.32\),

$$\delta n'_\nu = \begin{pmatrix} N\partial_\nu \xi^0 + N^3\partial_\nu \xi^0 + \mathcal{O}(\xi^2) \\ N\partial_\nu \xi^0 + \mathcal{O}(\xi^2) \end{pmatrix}, \quad (4.40)$$

and

$$\delta n'^\mu = \begin{pmatrix} -N\partial_\mu \xi^0 - \frac{\beta^i\partial_\mu \xi^i}{N} + \frac{\partial_\xi^0}{N} + \mathcal{O}(\xi^2) \\ N\partial_\mu \xi^i + N\beta^i\partial_\mu \xi^0 + N\partial_\mu \xi^0 - \frac{\beta^i\partial_\nu \xi^k}{N} + \frac{\partial_\xi^i}{N} + \mathcal{O}(\xi^2) \end{pmatrix} \quad (4.41)$$

respectively. If we then consider the quantity, $\delta K'_{\mu\nu}$, the infinitesimal difference between $K'_{\mu\nu}$ and $\bar{K}'_{\mu\nu}$, i.e.

$$K'_{\mu\nu} = \bar{K}'_{\mu\nu} + \delta K'_{\mu\nu}, \quad (4.42)$$

where, following the definition \(2.2\), we find $\delta K'_{\mu\nu}$,

$$\delta K'_{\mu\nu} = \delta \left( -\gamma_{(\mu}^i \nabla'_{\rho} n'_{\nu)} \right)$$

$$= - \left( \nabla'_{(\mu}(\delta n'_{\nu)}) + (\delta n'^\rho) n'_{(\mu} \nabla'_{\rho} n'_{\nu)} + (n'^\rho)(\delta n'_{(\mu}) \nabla'_{\rho} n'_{\nu)} \right). \quad (4.43)$$

Substituting \(4.40\) and \(4.41\) in \(4.43\) and using $\gamma_{\mu\nu} = g_{\mu\nu} + n_{\mu}n_{\nu}$, the hypersurface projection of the change in extrinsic curvature, $\delta K'_ij$, is given as,

$$\delta K'_{ij} = \frac{\partial(\delta n'_{ij})}{\partial x'^{(i)}} + (4)\Gamma^0_{ij}(\delta n'_{0}) + (4)\Gamma^k_{ij}(\delta n'_{k}) + \delta n'^0 n'_{(i} \Gamma_{0j}^0 n'_{j)} + \delta n'^k n'_{(i} \Gamma_{kj}^0 n'_{j)}$$

$$+ n'^0 \delta n'_{(i} \Gamma_{0j}^0 n'_{j)} + n'^k \delta n'_{(i} \Gamma_{kj}^0 n'_{j)}.$$

$^{25}$ Specifically, the 3-extrinsic curvature, $K'_{ij}$, given by the coordinate transformation \(4.33\), corresponds to a distinct re-formulation of the 3-foliation of spacetime. That is the 3-dimensional hypersurface $\Sigma'_t$, timelike unit vector $n'^a$, lapse function $N'$, and vector shift $\beta'_t$, of the new coordinate system, $\{x'^\mu\}$, are different physical entities to the corresponding $\Sigma_t$, $n^a$, $N$ and $\beta_t$ of the original coordinate system, $\{x^\mu\}$.
where \(^{(4)\Gamma}_{\nu^\rho}^\mu\) refers to the 4-dimensional Christoffel symbol. Finally, using \(n'_\mu = (-N', 0)\) and \(n''^\mu = 1/N'(1, -\beta''^i)\), we obtain at linear order in \(\xi^\mu\),

\[
\delta K'_{ij} = -N \partial_{ij} \xi^0 - \frac{\partial_0 \xi_0 (1 + N^2)}{2N} (\partial_j \beta_i + \partial_i \beta_j - \partial_0 \gamma_{ij}) + \frac{\partial_0 \xi_0 (1 + N^2) \beta^k}{2N} (\partial_j \gamma_{ki} + \partial_i \gamma_{kj} - \partial_k \gamma_{ij}) \\
+ \frac{\beta^k \partial_k \xi^0}{2N} (\partial_j \beta_i + \partial_i \beta_j - \partial_0 \gamma_{ij}) + \frac{N \gamma^{km} \partial_k \xi^0}{2N} (\partial_j \gamma_{mi} + \partial_i \gamma_{mj} - \partial_m \gamma_{ij}) \\
- \frac{\beta^k \beta^m \partial_k \xi^0}{2N} (\partial_j \gamma_{mi} + \partial_i \gamma_{mj} - \partial_m \gamma_{ij}) + \partial_i \xi^0 (\partial_j \beta_{ki} + \partial_k \gamma_{mj} - \partial_m \gamma_{kj}) + O(\xi^2).
\]

By considering terms up to and including \(O(\frac{1}{c^3})\), (4.44) simplifies to the recognizable form of the relationship (4.33),

\[
\delta K'_{ij} = \partial_{ij} \xi^0 + O \left( \frac{1}{c^2} \right).
\]  

Having proved the physical equivalence between the 2PN derived \(K_{ij}^{2\text{PN}}\) and the standard Bowen-York \(K_{ij}^{\text{BY}}\), it is then possible to use either the free data \((K_{ij}^{2\text{PN}}, K_{ij}^{2\text{PN}})\) or \((K_{ij}^{\text{BY}}, K \equiv 0)\). These results were given in both EC and CTS decompositions in Sections III A and III B respectively.

We finally provide complementary results to the PN free data presented in Sections III A and III B. Specifically, by assuming the widely used boundary conditions at spatial infinity, \(\Psi_{|r \to \infty} = 1\) and \(X^i_{|r \to \infty} = 0\), we solve for the constrained variables, \(X^i\) and \(\beta^i\), to 2PN order in the EC and CTS decompositions respectively:

1. **EC decomposition**

   a) Maximal hypersurface, \(K = 0\)

   i) \(\bar{\sigma} = 2N\)

   \[
   X^i = -\frac{Gm_1}{2c^3 r_1} (7v'_1 + n'_1(n_1 v_1)) + 1 \leftrightarrow 2 + O \left( \frac{1}{c^3} \right). \quad (4.46)
   \]

   ii) \(\bar{\sigma}^{\text{CTT}}\)

   \[
   X^i = -\frac{Gm_1}{4c^3 r_1} (7v'_1 + n'_1(n_1 v_1)) + 1 \leftrightarrow 2 + O \left( \frac{1}{c^3} \right). \quad (4.47)
   \]

   b) Mean curvature of \(K^{2\text{PN}}\)
i) \( \tilde{\sigma} = 2\tilde{N} \)

\[ X^i = -\frac{4Gm_1}{c^3r_1}v^i + 1 \leftrightarrow 2 + \mathcal{O}\left(\frac{1}{c^5}\right). \]  

(4.48)

ii) \( \tilde{\sigma}^{\text{CTT}} \)

\[ X^i = -\frac{2Gm_1}{c^3r_1}v^i + 1 \leftrightarrow 2 + \mathcal{O}\left(\frac{1}{c^5}\right). \]  

(4.49)

2. CTS decomposition

(a) Maximal hypersurface, \( K = 0 \)

\[ \beta^i = -\frac{Gm_1}{2c^3r_1} (7v^i_1 + n^i_1(n_1v_1)) + 1 \leftrightarrow 2 + \mathcal{O}\left(\frac{1}{c^5}\right). \]  

(4.50)

(b) Mean curvature with \( K^{2\text{PN}} \)

\[ \beta^i = -\frac{4Gm_1}{c^3r_1}v^i_1 + 1 \leftrightarrow 2 + \mathcal{O}\left(\frac{1}{c^5}\right). \]  

(4.51)

V. CONCLUSION

This work provides astrophysically realistic free data for binary black holes in numerical relativity, which are in agreement with 2PN results. Following the time-symmetric approach of [1], we propose a particular solution to the constraint equations in the form of the standard conformal decomposition of the spatial metric and extrinsic curvature. The solution presented here is shown to differ from the post-Newtonian metric in harmonic coordinates up to 2PN order by a coordinate transformation. The solution is also shown to differ at 2PN from the conformally-flat Bowen-York solution of the constraints, despite the singular nature of the proposed conformal metrics, \( \tilde{\gamma}_{ij} \) and \( \tilde{\gamma}^{\text{Dirac}}_{ij} \). We recall that the post-Newtonian metric is not only valid in the ‘near-zone’ of BBHs, but also arises from the re-expansion of a ‘global’ post-Minkowskian multipole expansion when \( c \to \infty \), which is equivalent to a far-zone expansion when \( r \to \infty \). In addition, the post-Newtonian masses \( m_1 \) and \( m_2 \) are introduced as coefficients of Dirac delta functions in the Newtonian density of point-like particles. Together with the formal energy and mass calculations for the time-symmetric instance [1], the interpretation of our solution as a perturbation of the Bowen-York solution
suggests that the post-Newtonian description of the black holes as delta-function singularities agrees with the physical masses of the Bowen-York black holes. The latter are computed by surface integrals at infinity and associated with Einstein-Rosen-like bridges.

We note, however, that our solution does not include the 2.5PN term of the metric, associated with Newtonian radiation reaction effects. Furthermore, although our solution exhibits characteristic 3PN features, we do not directly use the considerably more complex 3PN metric itself. In addition, we have only considered systems of two non-spinning black holes. However, spin effects are known to contribute directly to the gravitational waveform, and to the overall emission of energy and angular momentum of the system [70, 71, 72, 73]. Finally, it is important to note that further studies are required on the behavior of our solution in the vicinity of the black holes, providing an insight into the precise nature of the singularity, which is necessary for practical numerical implementation of the data.

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APPENDIX A: COMPARISON WITH THE KERR-SCHILD INITIAL DATA

One of the most widely-used set of initial data, which assumes a deviation from a conformally flat spacetime, is based on the superposition of two Kerr black holes in Kerr-Schild coordinates [31, 32]. When comparing with PN calculations, we find, however, that
the ‘physically realistic’ 2PN spatial metric, $g^{2\text{PN}}_{ij}$, disagrees with the free data constructed by superposing two Kerr-Schild metrics together. In particular, we show that the physical metric, $\gamma_{ij}^{\text{Kerr–Schild}}$, generated from a numerically-computed conformal factor, $\Psi^{\text{Kerr–Schild}}$, is inconsistent with post-Newtonian calculations at the 2PN level.

The Kerr-Schild spacetime metric for a single black hole of mass, $m$, and specific angular momentum, $a = j/m$ (where $j$ is the black hole’s angular momentum), is given by,

$$ds^2|_{\text{Kerr–Schild}} = \eta_{\mu\nu}dx^\mu dx^\nu + 2H(x^\alpha)l_\mu l_\nu dx^\mu dx^\nu, \quad (A1)$$

where $\eta_{\mu\nu}$ is the Minkowski flat-space metric, $H(x^\mu)$ represents a scalar function, and $l_\mu$ denotes the ingoing null vector (with respect to both the background and full metric) such that $\eta_{\mu\nu}l_\mu l_\nu = g_{\mu\nu}l_\mu l_\nu = 0$ (and hence, $l_\mu^2 = l_i l_i$). For a general Kerr-Schild black hole metric (expressed in Kerr’s original rectangular coordinates), $H(x^\mu)$ and $l_\mu$ are,

$$H = \frac{mr^3}{r^4 + (a \cdot x)^2}, \quad (A2)$$

and

$$l_\mu = \left(1, \frac{r x - a \times x + (a \cdot x)a/r}{r^2 + a^2}\right), \quad (A3)$$

where $r$ is given by,

$$r^2 = \frac{1}{2} (x^2 - a^2) + \sqrt{\frac{1}{4} (x^2 - a^2)^2 + (a \cdot x)^2}. \quad (A4)$$

From the spacetime metric (A1), we obtain the 3-spatial metric, $\gamma_{ij}$, within the ADM decomposition,

$$\gamma_{ij}^{\text{Kerr–Schild}} = \delta_{ij} + 2Hl_i l_j, \quad (A5)$$

together with the ADM gauge variables $\beta_i = 2Hl_0 l_i$ and $\alpha = \frac{1}{\sqrt{1 + 2Hl_0^2}}$. From (2.4), the extrinsic curvature $K_{ij}^{\text{Kerr–Schild}}$ is thus given as,

$$K_{ij}^{\text{Kerr–Schild}} = \frac{1}{2\alpha} \left[ \nabla_j \beta_i + \nabla_i \beta_j - \partial_t \gamma_{ij}^{\text{Kerr–Schild}} \right]. \quad (A6)$$

The Kerr-Schild conformal metric of two black holes, $\tilde{\gamma}_{ij}^{\text{Kerr–Schild}}$, is generated from the ‘superposition’ of two Kerr-Schild coordinate systems (A5), each describing a single black hole (see Eqn. (28) in [31] and Eqn. (21) in [32]), i.e.

$$\tilde{\gamma}_{ij}^{\text{Kerr–Schild}} = \delta_{ij} + 2 \left[ H(r_1) l_i l_j + H(r_2) l_i l_j \right], \quad (A7)$$
where the indices 1 and 2 label the two black holes. Similarly, the mean curvature is given as,

$$K_{\text{Kerr-Schild}} = 1(K^i)_{\text{Kerr-Schild}} + 2(K^i)_{\text{Kerr-Schild}},$$  \hspace{1cm} (A8)$$

and the conformal symmetric trace-free extrinsic curvature is,

$$\tilde{A}_{ij}^{\text{Kerr-Schild}} = (\tilde{\gamma}_{k(i})^{\text{Kerr-Schild}} [1(K^k)_{\text{Kerr-Schild}} - \frac{1}{3} \delta_{ij} \frac{1}{2} (K^i)_{\text{Kerr-Schild}}] + 2(K^j)_{\text{Kerr-Schild}} - \frac{1}{3} \delta_{ij} \frac{2}{2} (K^i)_{\text{Kerr-Schild}}],$$  \hspace{1cm} (A9)$$

where

$$1(K^k)_{\text{Kerr-Schild}} = \frac{1}{2}(\gamma^{k})^{\text{Kerr-Schild}} \left[ \nabla_j 1\beta^i + \nabla_i 1\beta_j - \partial_i 1(\gamma_{ij})^{\text{Kerr-Schild}} \right]$$

and

$$1(\gamma_{ij})^{\text{Kerr-Schild}} = 2 \frac{H(r_1)}{r_1} 1l_i 1l_j;$$

see \[32\] for details. Note that for simplicity, we have not included the ‘attenuation functions’ \(B_1\) and \(B_2\), introduced in \[32, 33\].

For illustrative purposes, we consider here the simplest instance of two non-spinning black holes (i.e. \(a = 0\)), where the Kerr-Schild 3-conformal metric is given explicitly as,

$$\tilde{\gamma}_{ij}^{\text{Kerr-Schild}} = \delta_{ij} + \frac{2GM_1}{c^2r_1} n_1^i n_1^j + \frac{2GM_2}{c^2r_2} n_2^i n_2^j,$$  \hspace{1cm} (A10)$$

and the Hamiltonian constraint \(2.9\) is of the form,

$$\tilde{\Delta} \psi^{\text{Kerr-Schild}} = \frac{1}{8}(\tilde{R}(\psi^{\text{Kerr-Schild}}) + \frac{1}{12}(K^{\text{Kerr-Schild}})^2 \right) - \frac{7}{8}(\tilde{A}_{ij})^{\text{Kerr-Schild}} \tilde{A}_{ij}^{\text{Kerr-Schild}}$$  \hspace{1cm} (A11)$$

where \(K^{\text{Kerr-Schild}}\) and \(\tilde{A}_{ij}^{\text{Kerr-Schild}}\) are of order \(O(1/c^3)\) using \(A8\) and \(A9\).

Let us now assume that the Kerr-Schild conformal factor, \(\psi^{\text{Kerr-Schild}}\), at the 1PN order, is given by,

$$\psi^{\text{Kerr-Schild}} = 1 + \frac{\gamma}{c^2} + \left(\frac{1}{c^4}\right),$$  \hspace{1cm} (A12)$$

which results in an explicit expression for the function \(Y\) from \(A11\),

$$Y = -\frac{GM_1}{2r_1} - \frac{GM_2}{2r_2} + \frac{AGM_1}{r_1} + \frac{BGM_2}{r_2},$$  \hspace{1cm} (A13)$$

where \(\sim \frac{AGM_1}{r_1}\) and \(\sim \frac{BGM_2}{r_2}\) are additional ‘homogeneous’ terms, which occur when solving \(A12\). Note that when \(\psi^{\text{Kerr-Schild}} \equiv \psi^{B-L}\), the constants \(A = B = 1\), where \(\psi^{B-L}\) is the Brill-Lindquist conformal factor given by (4.16).

By substituting \(A12\) and \(A13\) into the conformal relationship, \(\tilde{\gamma}_{ij}^{\text{Kerr-Schild}} = (\psi^{\text{Kerr-Schild}})^4 \gamma_{ij}^{\text{Kerr-Schild}}\), we find that constants \(A = B = 1/2\) in \(A13\) for the following...
isometric relationship to be true at 1PN order,

\[ \gamma_{ij}^{\text{Kerr–Schild}} = g_{ij}^{\text{1PN}} + \delta_i \varsigma_j + \delta_j \varsigma_i, \tag{A14} \]

where \( g_{ij}^{\text{1PN}} \) is the 1PN spatial metric in harmonic coordinates given by Eqn. (7.2c) in [56].

The infinitesimal spatial gauge vector, \( \varsigma_i \), is uniquely determined as,

\[ \varsigma_i = -\frac{Gm_1}{c^2} n_i^1 - \frac{Gm_2}{c^2} n_i^2 + \mathcal{O} \left( \frac{1}{c^4} \right). \tag{A15} \]

Using \( A = B = 1/2 \) in (A13) and inserting \( \Psi_{\text{Kerr–Schild}} \) into (2.8), it is immediately apparent that the physical metric, \( \gamma_{ij}^{\text{Kerr–Schild}} \), is not isometric with \( g_{ij}^{\text{2PN}} \) - the 2PN spatial metric in harmonic coordinates given by Eqn. (7.2c) in [56]. More specifically, \( \tilde{\gamma}_{ij}^{\text{Kerr–Schild}} \) does not contain any ‘interaction’ terms \( \sim m_1 m_2 \) of the two black holes. Notably, there are no terms involving the ‘interaction’ function \( g \), where we recall that \( g \) and its associated derivatives (such as (3.9) and (3.10)) are characteristic of post-Newtonian results at 2PN order and higher. The absence of such terms in \( \tilde{\gamma}_{ij}^{\text{Kerr–Schild}} \) is a direct consequence from its construction as a linear superposition of two Kerr-Schild coordinate systems. Note that it is impossible to incorporate all the 2PN features of \( g_{ij}^{\text{2PN}} \) into higher order terms of the conformal factor \( \Psi_{\text{Kerr–Schild}} \).

We, therefore, conclude that the Kerr-Schild conformal metric is incompatible with the inspiral physics described accurately by 2PN results.

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