Comparing post-Newtonian and numerical relativity precession dynamics

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Binary black-hole systems are expected to be important sources of gravitational waves for upcoming gravitational-wave detectors. If the spins are not colinear with each other or with the orbital angular momentum, these systems exhibit complicated precession dynamics that are imprinted on the gravitational waveform. We develop a new procedure to match the precession dynamics computed by post-Newtonian (PN) theory to those of numerical binary black-hole simulations in full general relativity. For numerical relativity (NR) simulations lasting approximately two precession cycles, we find that the PN and NR predictions for the directions of the orbital angular momentum and the spins agree to better than ~1° with NR during the inspiral, increasing to 5° near merger. Nutation of the orbital plane on the orbital time scale agrees well between NR and PN, whereas nutation of the spin direction shows qualitatively different behavior in PN and NR. We also examine how the PN equations for precession and orbital-phase evolution converge with PN order, and we quantify the impact of various choices for handling partially known PN terms.

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I. INTRODUCTION

Binary black-hole systems are expected to be important sources of gravitational waves for upcoming gravitational-wave detectors like Advanced LIGO [1] and Virgo [2]. Accurate predictions of the gravitational waveforms emitted by such systems are important for detection of gravitational waves and for parameter estimation of any detected binary [3]. When either black hole carries spin that is not aligned with the orbital angular momentum, there is an exchange of angular momentum between the components of the system, leading to complicated dynamical behavior. Figure 1 exhibits the directions of the various angular momenta in several simulations described in this paper. This behavior is imprinted on the emitted waveforms [4–6], making them more feature-rich than waveforms from aligned-spin BBH systems or nonspinning BBH systems. In order to model the waveforms accurately, then, we need to understand the dynamics.

The orbital-phase evolution of an inspiraling binary, the precession of the orbital angular momentum and the black-hole spins, and the emitted gravitational waveforms can be modeled with post-Newtonian theory [7], a perturbative solution of Einstein’s equations in powers of \( v/c \), the ratio of the velocity of the black holes to the speed of light. Such post-Newtonian waveforms play an important role in the waveform modeling for ground-based interferometric gravitational-wave detectors (see, e.g., [8]).

For nonspinning and aligned-spin BBH, a large number of comparisons between PN and NR have been performed, among them [9–19]. For these nonprecessing systems, gravitational wave phasing reduces to only one degree of freedom, generally taken to be the argument of the complex-valued (2,2) mode of the emitted gravitational radiation. Because phasing is of high importance for matching filtering, PN-NR comparisons for nonprecessing binaries have focused on the accumulated phase differences in the dominant (2,2) mode of the gravitational waveform. It was found that the PN error due to truncation of the PN series at some finite order (typically 3.5PN) can be quite large, especially at mass-ratios \( \gtrsim 5 \) and for spinning black holes. The resulting phase error was identified as one of the dominant limitations of waveform modeling for nonprecessing BBH [14,17,20–23]. By coincidence, the uncontrolled higher-order terms in PN approximants can sometimes be close to the correct, unknown values. Comparisons that rely on only one PN approximant are therefore prone to underestimate the error of PN. The best known case for this behavior are equal mass, nonspinning BBH, where the TaylorT4 approximant appears significantly more accurate than other Taylor approximants [9,11].

Precessing waveform models (e.g., [6,24–27]) depend on the orbital phase evolution and the precession dynamics. Therefore, it is important to quantify the accuracy of the post-Newtonian approximation for modeling the precession dynamics itself, and the orbital-phase evolution of
precessing binaries. The first such comparison was performed by Campanelli et al [28] finding fairly good agreement between PN and NR, with phase differences of about a cycle close to merger. They also found that 3.5 PN approximant performed significantly better than 2.5 PN. Lousto and Zlochower [29] studied the precession dynamics of a long numerical relativity simulation undergoing a reversal of the black hole spin direction, and found excellent agreement between NR and PN until close to merger.

In 2013, the SXS Collaboration published numerical-relativity solutions to the full Einstein equations for precessing BBH systems [30]. These simulations cover ≳ 30 orbits and up to two precession cycles. Therefore, they offer a novel opportunity to systematically quantify the accuracy of the post-Newtonian precession equations, the topic of this paper. The first such comparisons based on the SXS catalog were made in [26,30]. Ref. [26] found that Taylor T4 model disagreed with the NR data much more than the spinning EOB model. The PN precession equations used in [26], however, were only leading order, and it remained unclear whether the disagreement of Taylor T4 arises because of the low order of precession equations, or more general deficiencies of PN. The preliminary comparison of two precessing cases in [30] demonstrated good agreement of spin and angular momentum precession and motivated the current work. That study is expanded and refined here to include higher-order PN terms in the precession equations and the evolution of the orbital frequency.

While this paper focuses on comparison of the orbital dynamics (angular momenta directions and orbital phase), in order to disentangle different aspects of the precessing BBH inspirals, some authors have performed comparisons of the emitted waveforms [24,25,28]. Tarrachini et al. [25] computed the unfaithfulness of the SEOBNRv3 model for a $q = 5, \chi_1 = 0.5, \chi_2 = 0$ (see case q5_0.5x in Table I) and found to be less than 3% which would translate to negligible losses in detection rate. Hannam et al. [24] computed fitting factors between PN-NR hybrid models and a phenomenological precessing PhenomP model and found fitting factors $\geq 0.965$ for most sky orientations for cases with $q \leq 3$, in contrast to lower fitting factors obtained when using the nonprecessing PhenomC [31] model.
TABLE I. Numerical relativity simulations utilized here. SXS ID refers to the simulation number in Ref. [30], $q = m_1/m_2$ is the mass ratio, $\chi_{1,2}$ are the dimensionless spins, given in coordinates where $\hat{n}(t = 0) = \hat{x}$, $\hat{\epsilon}(t = 0) = \hat{z}$. $D_0$, $\Omega_0$ and $e$ are the initial coordinate separation, the initial orbital frequency, and the orbital eccentricity, respectively. The first block lists the precessing runs utilized, where $\chi_{1,r} = (-0.18, -0.0479, -0.0378)$ and $\chi_{2,r} = (-0.0675, 0.0779, -0.357)$. The second block indicates 31 further precessing simulations used in Fig. 13, and the last block lists the aligned spin systems for orbital phase comparisons.

<table>
<thead>
<tr>
<th>Name</th>
<th>SXS ID</th>
<th>$q$</th>
<th>$\chi_1$</th>
<th>$\chi_2$</th>
<th>$D_0/M$</th>
<th>$m\Omega_0$</th>
<th>$e$</th>
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<tr>
<td>q1_0.5x</td>
<td>0003</td>
<td>1.0</td>
<td>(0.5,0,0,0)</td>
<td>(0,0,0)</td>
<td>19</td>
<td>0.01128</td>
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<td>1.5</td>
<td>(0.5,0.0,0)</td>
<td>(0,0,0)</td>
<td>16</td>
<td>0.01443</td>
<td>$&lt; 2 \times 10^{-4}$</td>
</tr>
<tr>
<td>q3_0.5x</td>
<td>0034</td>
<td>3.0</td>
<td>(0.5,0.0,0)</td>
<td>(0,0,0)</td>
<td>14</td>
<td>0.01743</td>
<td>$&lt; 2 \times 10^{-4}$</td>
</tr>
<tr>
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<td>(0.5,0.0,0)</td>
<td>(0,0,0)</td>
<td>15</td>
<td>0.01579</td>
<td>0.002</td>
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<tr>
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<td>(0.52,0,0.3)</td>
<td>(0.52,0,0.3)</td>
<td>15.3</td>
<td>0.01510</td>
<td>0.003</td>
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<tr>
<td>q1.97_random</td>
<td>0146</td>
<td>1.97</td>
<td>$\chi_{1,r}$</td>
<td>$\chi_{2,r}$</td>
<td>15</td>
<td>0.01585</td>
<td>$&lt; 10^{-4}$</td>
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<tr>
<td>31 random runs</td>
<td></td>
<td></td>
<td>$\chi_1 \leq 0.5$</td>
<td>$\chi_2 \leq 0.5$</td>
<td>15</td>
<td>$\approx 0.0159$</td>
<td>$[10^{-4}, 10^{-3}]$</td>
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<tr>
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<td>(0,0,0.5)</td>
<td>(0,0,0)</td>
<td>19</td>
<td>0.01127</td>
<td>0.0003</td>
</tr>
<tr>
<td>q1,-0.5z</td>
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<td>19</td>
<td>0.01131</td>
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<td>q1.5,-0.5z</td>
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<td>16</td>
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<td>(0,0,0)</td>
<td>15</td>
<td>0.01591</td>
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<td>0065</td>
<td>8.0</td>
<td>(0,0,0.5)</td>
<td>(0,0,0)</td>
<td>13</td>
<td>0.01922</td>
<td>0.004</td>
</tr>
<tr>
<td>q8,-0.5z</td>
<td>0064</td>
<td>8.0</td>
<td>(0,0,0.5)</td>
<td>(0,0,0)</td>
<td>13</td>
<td>0.01954</td>
<td>0.0005</td>
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In this paper, we develop a new technique to match the initial conditions of post-Newtonian dynamics to a numerical relativity simulation. We then use this technique to study the level of agreement between the post-Newtonian precession equations and the numerical simulations. The agreement is remarkably good, the directions of orbital angular momentum and spin axes in post-Newtonian theory reproduces the numerical simulations usually to better than 1 degree. We also investigate nutation effects on the orbital time scale that are imprinted both in the orbital angular momentum and the spin-directions. For the orbital angular momentum, NR and PN yield very similar nutation features, whereas for the spin direction, nutation is qualitatively different in PN and the investigated NR simulations. Considering the orbital-phase evolution, we find that the disagreement between post-Newtonian orbital phase and numerical relativity simulation is comparable to the aligned-spin case. This implies that the orbital phase evolution will remain an important limitation for post-Newtonian waveforms even in the precessing case. Finally, we study the convergence with post-Newtonian order of the precession equations, and establish very regular and fast convergence, in contrast to post-Newtonian orbital phasing.

This paper is organized as follows: Section II describes the post-Newtonian expressions utilized, the numerical simulations, how we compare PN and NR systems with each other, and how we determine suitable “best-fitting” PN parameters for a comparison with a given NR simulation. Section III presents our results, starting with a comparison of the precession dynamics in Sec. III A, and continuing with an investigation in the accuracy of the orbital phasing in Sec. III B. The following two sections study the convergence of the PN precession equations and the impact of ambiguous choices when dealing with incompletely known spin-terms in the PN orbital phasing. Section III E, finally, is devoted to some technical numerical aspects, including an investigation into the importance of the gauge conditions used for the NR runs. We close with a discussion in Sec. IV. The appendices collect the precise post-Newtonian expressions we use and additional useful formulae about quaternions.

II. METHODOLOGY

A. Post-Newtonian Theory

Post-Newtonian (PN) theory is an approximation to general relativity in the weak-field, slow-motion regime, characterized by the small parameter $c \sim (v/c)^2 \sim \frac{Gm}{rc^2}$, where $m$, $v$, and $r$ denote the characteristic mass, velocity, and size of the source, $c$ is the speed of light, and $G$ is Newton’s gravitational constant. For the rest of this paper, the source is always a binary black-hole system with total mass $m$, relative velocity $v$ and separation $r$, and we use units where $G = c = 1$.

Restricting attention to quasispherical binaries in the adiabatic limit, the local dynamics of the source can be split into two parts: the evolution of the orbital frequency, and the precession of the orbital plane and the spins. The leading-order precession effects [32] and spin contributions to the evolution of the orbital frequency [33,34] enter...
post-Newtonian dynamics at the 1.5 PN order (i.e., \(e^{3/2}\)) for spin-orbit effects, and 2 PN order for spin-spin effects. We also include nonspin terms to 3.5 PN order \([7]\), the spin-orbit terms to 4 PN order \([35]\), spin-spin terms to 2 PN order \([34]\).\(^1\) For the precession equations, we include the spin-orbit contributions to next-to-next-to-leading order, corresponding to 3.5 PN \([37]\). The spin-spin terms are included at 2 PN order.\(^2\)

1. Orbital dynamics

Following earlier work (e.g., Ref. \([34]\)) we describe the precessing BH binary by the evolution of the orthonormal triad \((\hat{n}, \hat{\lambda}, \hat{\epsilon})\), as indicated in Fig. 2: \(\hat{n}\) denotes the unit separation vector between the two compact objects, \(\hat{\epsilon}\) is the normal to the orbital plane and \(\hat{\lambda} = \hat{\epsilon} \times \hat{n}\) completes the triad. This triad is time-dependent, and is related to the constant inertial triad \((\hat{x}, \hat{y}, \hat{z})\) by a time-dependent rotation \(R_f\), as indicated in Fig. 2. The rotation \(R_f\) will play an important role in Sec. II C. The orbital triad obeys the following equations:

\[
\begin{align*}
\frac{d\hat{\epsilon}}{dt} &= \sigma \hat{n} \times \hat{\epsilon}, \\
\frac{d\hat{n}}{dt} &= \Omega \hat{\lambda}, \\
\frac{d\hat{\lambda}}{dt} &= -\Omega \hat{n} + \sigma \hat{\epsilon}.
\end{align*}
\]

Here, \(\Omega\) is the instantaneous orbital frequency and \(\sigma\) is the precession frequency of the orbital plane.

The dimensionless spin vectors \(\vec{\chi}_i = \vec{S}_i / m_i^2\) also obey precession equations:

\[
\begin{align*}
\frac{d\vec{\chi}_1}{dt} &= \vec{\Omega}_1 \times \vec{\chi}_1, \\
\frac{d\vec{\chi}_2}{dt} &= \vec{\Omega}_2 \times \vec{\chi}_2.
\end{align*}
\]

The precession frequencies \(\vec{\Omega}_{1,2}, \sigma\) are series in the PN expansion parameter \(e\); their explicit formulas are given in Appendix A.

The evolution of the orbital frequency is derived from energy balance:

\[
\frac{dE}{dt} = -\mathcal{F},
\]

where \(E\) is the energy of the binary and \(\mathcal{F}\) is the gravitational-wave flux. \(E\) and \(\mathcal{F}\) are PN series depending on the orbital frequency \(\Omega\), the vector \(\hat{\epsilon}\), and the BH spins \(\vec{\chi}_1, \vec{\chi}_2\). Their explicit formulas are given in Appendix A. In terms of \(x \equiv (m \Omega)^{2/3} \sim e\), Eq. (3) becomes

\[
\frac{dx}{dt} = -\frac{\mathcal{F}}{dE/dx},
\]

where the right-hand side is a ratio of 2 PN series.

There are several well known ways of solving Eq. (4), which lead to different treatment of uncontrolled higher-order PN terms—referred to as the Taylor T1 through T5 approximants \([45,46]\). The most straightforward approach is to evaluate the numerator and denominator of Eq. (4) and then solve the resulting ordinary differential equation numerically, which is the Taylor T1 approximant. Another approach is to reexpand the ratio \(\mathcal{F}/(dE/dx)\) in a new power series in \(x\), and then truncate at the appropriate order. This gives the Taylor T4 approximant. Finally, one can expand the inverse of the right-hand side of Eq. (4) in a new power series in \(x\), truncate it at the appropriate order, and then substitute the inverse of the truncated series into the right-hand side in Eq. (4). This last approach, known as the Taylor T5 approximant \([46]\), has been introduced fairly recently.

2. Handling of spin terms

When constructing Taylor approximants that include the reexpansion of the energy balance equation, the handling of spin terms becomes important. In particular, terms of
quadratic and higher order in spins, such as $(\mathbf{S}_i)^2$, appear in the evolution of the orbital frequency at 3 PN and higher orders. These terms arise from lower-order effects and represent incomplete information, since the corresponding terms are unknown in the original power series for the binding energy $E$ and the flux $\mathcal{F}$,

$$E(x) = -\frac{1}{2} m u x \left(1 + \sum_{k=2}^{5} a_k x^{k/2}\right),$$

$$\mathcal{F}(x) = \frac{32}{5} \nu^2 x^5 \left(1 + \sum_{k=2}^{5} b_k x^{k/2}\right),$$

where $m = m_1 + m_2$ and $\nu = m_1 m_2 / m^2$, and $m_{1,2}$ are the individual masses.

In these expansions, the spin-squared terms come in at 2 PN order and thus appear in $a_4$ and $b_4$, cf. Eqs. (A18) and (A24). Then, in the re-expansion series of Taylor T4,

$$S = -\frac{\mathcal{F}}{dE/dx} = \frac{64u}{5m} x^5 \left(1 + \sum_{k=2}^{5} s_k x^{k/2}\right),$$

the coefficients $s_k$ can be recursively determined, e.g.

$$s_4 = b_4 - 3a_4 - 2s_2a_2,$$

$$s_6 = b_6 - \left(4a_6 + 3s_2a_4 + \frac{5}{2} s_3a_3 + 2s_4a_2\right).$$

Thus, the spin-squared terms in $a_4$ and $b_4$ will induce spin-squared terms at 3PN order in $s_6$. The analogous conclusion holds for Taylor T5. These spin-squared terms are incomplete as the corresponding terms in the binding energy and flux (i.e. in $a_6$ and $b_6$) are not known.

This re-expansion has been handled in several ways in the literature. For example, Nitz et al. [23] include only terms which are linear in spin beyond 2 PN order. On the other hand, Santamaría et al. [31] keep all terms in spin arising from known terms in $E$ and $\mathcal{F}$. In the present work, we also keep all terms up to 3.5 PN order, which is the highest order to which nonspin terms are completely known. Similarly, we include all terms when computing the precession frequency (see A 2). We investigate the impact of different spin-truncation choices in Sec. III D, along with the impact of partially known 4 PN spin terms.

**B. Numerical relativity simulations**

To characterize the effectiveness of PN theory in reproducing NR results, we have selected a subset of 16 simulations from the SXS waveform catalog described in Ref. [30]. Our primary results are based on six precessing simulations and a further ten nonprecessing ones for cross-comparisons. To check for systematic effects, we use a further 31 precessing simulations with random mass ratios and spins. The parameters of these runs are given in Table I. They were chosen to represent various degrees of complexity in the dynamics: (i) precessing versus nonprecessing simulations, the latter with spins parallel or antiparallel to \( \mathbf{\hat{e}} \), (ii) one versus two spinning black holes, (iii) coverage of mass ratio from $q = 1$ to $q = 8$, (iv) long simulations that cover more than a precession cycle, and (v) a variety of orientations of $\mathbf{\hat{\gamma}}_1$, $\mathbf{\hat{\gamma}}_2$, $\mathbf{\hat{\gamma}}$. Figure 1 shows the precession cones of the normal to the orbital plane and the spins for the six primary precessing cases in Table I. The PN data were computed using the Taylor T4 3.5 PN approximant.

The simulations from the catalog listed in Table I were run with numerical methods similar to [47]. A generalized harmonic evolution system [48–51] is employed, and the gauge is determined by gauge source functions $H_\alpha$. During the inspiral phase of the simulations considered here, $H_\alpha$ is kept constant in the comoving frame, cf. [11,52,53]. About 1.5 orbits before merger, the gauge is changed to damped harmonic gauge [54–56]. This gauge change happens outside the focus of the comparisons presented here.

The simulation $q5_0.5x$ analyzed here is a rerun of the SXS simulation SXS:BBH:0058 from Ref. [31]. We performed this rerun for two reasons: First, SXS:BBH:0058 changes to damped harmonic gauge in the middle of the inspiral, rather than close to merger as all other cases considered in this work. Second, SXS:BBH:0058 uses an unsatisfactorily low numerical resolution during the calculation of the black hole spins. Both these choices leave noticeable imprints on the data from SXS:BBH:0058, and the rerun $q5_0.5x$ allows us to quantify the impact of these deficiencies. We discuss these effects in detail in Secs. III E 2 and III E 3. The rerun $q5_0.5x$ analyzed here is performed with improved numerical techniques. Most importantly, damped harmonic gauge is used essentially from the start of the simulation, $t \gtrsim 100M$. The simulation $q5_0.5x$ also benefits from improved adaptive mesh refinement [57] and improved methods for controlling the shape and size of the excision boundaries; the latter methods are described in Sec. II B of Ref. [58].

We have performed convergence tests for some of the simulations; Sec. III E will demonstrate with Fig. 19 that numerical truncation error is unimportant for the comparisons presented here.

**C. Characterizing precession**

The symmetries of nonprecessing systems greatly simplify the problem of understanding the motion of the binary. In a nonprecessing system, the spin vectors are essentially constant, and two of the rotational degrees of freedom are eliminated in the binary’s orbital elements. Assuming quasicircular orbits, the entire system can be
described by the orbital phase $\Phi$, which can be defined as the angle between $\hat{n}$ and $\hat{x}$. In post-Newtonian theory the separation between the black holes can be derived from $d\Phi/dt$. Thus comparison between post-Newtonian and numerical orbits, for example, reduces entirely to the comparison between $\Phi_{\text{PN}}$ and $\Phi_{\text{NR}}$ [11,59]. For precessing systems, on the other hand, the concept of an orbital phase is insufficient; $\Phi$ could be thought of as just one of the three Euler angles. We saw in Sec. II A 1 that the orbital dynamics of a precessing system can be fairly complex, involving the triad $(\hat{n}, \hat{\lambda}, \hat{\chi})$ or equivalently the frame rotor $R_{\ell}$, as well as the two spin vectors $\hat{\chi}_1$ and $\hat{\chi}_2$—each of which is, of course, time dependent. When comparing post-Newtonian and numerical results, we need to measure differences between each of these quantities in their respective systems.

To compare the positions and velocities of the black holes themselves, we can condense the information about the triads into the quaternion quantity [60]

$$R_{\Delta} := R_{\ell, \text{PN}}^{-1} R_{\ell, \text{NR}}^{-1},$$

which represents the rotation needed to align the PN frame with the NR frame. This is a geometrically meaningful measure of the relative difference between two frames. We can reduce this to a single real number by taking the magnitude of the logarithm of this quantity, defining the angle,

$$\Phi_{\Delta} := 2|\log R_{\Delta}|.$$  

This measure has various useful qualities. It is invariant, in the sense that any basis frame used to define $R_{\ell, \text{PN}}$ and $R_{\ell, \text{NR}}$ will result in the same value of $\Phi_{\Delta}$. It conveniently distills the information about the difference between the frames into a single value, but is also nondegenerate in the sense that $\Phi_{\Delta} = 0$ if and only if the frames are identical. It also reduces precisely to $\Phi_{\text{PN}} - \Phi_{\text{NR}}$ for nonprecessing systems; for precessing systems it also incorporates contributions from the relative orientations of the orbital planes.

Despite these useful features of $\Phi_{\Delta}$, it may sometimes be interesting to use different measures, to extract individual components of the binary evolution. For example, Eq. (1a) describes the precession of the orbital plane. When comparing this precession for two approaches, a more informative quantity than $\Phi_{\Delta}$ is simply the angle between the $\hat{\chi}$ vectors in the two systems:

$$\angle(L) = \cos^{-1}(\hat{\chi}_{\text{PN}} \cdot \hat{\chi}_{\text{NR}}).$$

Similarly, we will be interested in understanding the evolution of the spin vectors, as given in Eqs. (2). For this purpose, we define the angles between the spin vectors:

$$\angle(L) = \cos^{-1}(\hat{\chi}_{\text{PN}} \cdot \hat{\chi}_{\text{NR}}).$$

We will use all four of these angles below to compare the post-Newtonian and numerical orbital elements.

**D. Matching post-Newtonian to numerical relativity**

When comparing PN theory to NR results, it is important to ensure that the initial conditions used in both cases represent the same physical situation. We choose a particular orbital frequency $\Omega$ and use the NR data to convert it to a time $t_m$. To initialize a PN evolution at $t_m$, we need to specify

$$q, \chi_1, \chi_2,$$

$$\hat{\chi}, \hat{n}, \hat{\chi}_1, \hat{\chi}_2,$$

$$\Omega.$$ 

The quantities (14) are conserved during the PN evolution. The quantities (15) determine the orientation of the binary and its spins relative to the inertial triad $(\hat{x}, \hat{y}, \hat{z})$. The orbital frequency $\Omega$ in Eq. (16), finally, parameterizes the separation of the binary at $t_m$. The simplest approach is to initialize the PN evolution from the respective quantities in the initial data of the NR evolution. This would neglect initial transients in NR data as in, e.g., Fig. 1 of Ref. [53]. These transients affect the masses and spins of the black holes; so any further PN-NR comparisons would be comparing slightly different physical configurations. The NR transients decay away within the first orbit of the NR simulation, so one can consider initializing the PN evolution from NR at a time after the NR run has settled down. However, the generally nonzero (albeit very small) orbital eccentricity in the NR simulation can lead to systematic errors in the subsequent comparison as pointed out in Ref. [11].

Therefore, we use time-averaged quantities evaluated after the initial transients have vanished. In particular, given a numerical relativity simulation, we set the PN variables listed in Eq. (14) to their numerical relativity values after junk radiation has propagated away.

The remaining nine quantities Eqs. (15) and (16) must satisfy the constraint $\hat{\chi} \cdot \hat{n} = 0$. We determine them with constrained minimization by first choosing an orbital frequency interval $[\Omega_m, \Omega_m + \delta \Omega / 2]$ of width $\delta \Omega$. Computing the corresponding time interval $[t_i, t_f]$ in
the NR simulation, we define the time average of any quantity $Q$ by

$$\langle Q \rangle = \frac{1}{t_f - t_i} \int_{t_i}^{t_f} Q dt.$$  

(17)

Using these averages, we construct the objective functional $S$ as

$$S = \langle (\angle L)^2 \rangle + \langle (\angle \chi_1)^2 \rangle + \langle (\angle \chi_2)^2 \rangle + \langle (\angle n)^2 \rangle + \langle (\Delta \Omega)^2 \rangle$$  

(18)

where $\Delta \Omega = (\Omega_{PN} - \Omega_{NR})/\Omega_{NR}$, and $\angle n$ is defined analogously to Eq. (12). When a spin on the black holes is below $10^{-5}$ the corresponding term is dropped from Eq. (18).

The objective functional is then minimized using the SLSQP algorithm [61,62] to allow for constrained minimization. In Eq. (18) we use equal weights for each term; other choices of the weights do not change the qualitative picture that we present.

The frequency interval $[\Omega_m \pm \delta \Omega/2]$ is chosen based on several considerations. First it is selected after junk radiation has propagated away. Secondly, it is made wide enough so that any residual eccentricity effects average out. Finally, we would like to match PN and NR as early as possible. But since we want to compare various cases to each other, the lowest possible matching frequency will be limited by the shortest NR run (case q0.5x). Within these constraints, we choose several matching intervals, in order to estimate the impact of the choice of matching interval on our eventual results. Specifically, we use three matching frequencies

$$m\Omega_m \in \{0.021067, 0.021264, 0.021461\},$$  

(19)

and employ four different matching windows for each, namely

$$\delta \Omega / \Omega_m \in \{0.06, 0.08, 0.1, 0.12\}.$$  

(20)

These frequencies correspond approximately to the range between 10–27 orbits to merger depending on the parameters of the binary, with the lower limit for the case q1.97_random and the upper for q5_0.5x.

Matching at multiple frequencies and frequency windows allows an estimate on the error in the matching and also ensures that the results are not sensitive to the matching interval being used. In this article, we generally report results that are averaged over the 12 PN-NR comparisons performed with the different matching intervals. We report error bars ranging from the smallest to the largest result among the 12 matching intervals. As examples, Fig. 3 shows $\Phi_\Delta$ as a function of time to merger $t_{merge}$ for the cases q1.97_random and q5_0.5x for all the matching frequencies and intervals, as well as the average result and an estimate of the error. Here $t_{merge}$ is the time in the NR simulation when the common horizon is detected.

**III. RESULTS**

**A. Precession comparisons**

We apply the matching procedure of Sec. II D to the precessing NR simulations in Table I. PN–NR matching is always performed at the frequencies given by Eq. (19) which are the lowest feasible orbital frequencies across all cases in Table I. Figure 1 shows the precession cones for the normal to the orbital plane $\hat{L}$ and the spins $\hat{\chi}_1, \hat{\chi}_2$. As time progresses, $\hat{L}$ and $\hat{\chi}_1, \hat{\chi}_2$ undergo precession and nutation, and the precession cone widens due to the emission of gravitational radiation. Qualitatively, the PN results seem to follow the NR results well, until close to merger.

We now turn to a quantitative analysis of the precession dynamics, establishing first that the choice of Taylor approximant is of minor importance for the precession dynamics. We match PN dynamics to the NR simulations q5_0.5x and q1_0.5x for the Taylor approximants T1, T4...
Motivated by the separation of time scales, orbit-averaged PN precession equations were developed and widely used in literature (see e.g. [4,34,64]). Because these equations eliminate the orbital time scale, they are much easier to integrate. For example, the SpinTaylorT4 model of the LIGO Algorithm Library [65] utilizes the leading order orbit-averaged precession equations [66]. As an example, we construct and match orbit-averaged and full PN precession equations at leading order in spin-orbit and spin-spin couplings (i.e., the precession equations are at 2 PN order). Figure 7 presents $\chi$ and $\dot{\ell}$ for the case q5_0.5x for the run q5_0.5x, we compute the angle $\angle \chi$ between the averaged spin vectors, $\chi_{\text{PN}}$ and $\chi_{\text{NR}}$. This angle is plotted in Fig. 6 where results only for the Taylor T1 approximant are shown, and for only one matching interval specified by $m\Omega_m = 0.0210597$ and $\delta\Omega/\Omega_m = 0.1$. The orbit-averaged spin directions $\chi_{\text{NR/\text{PN}}}$ agree significantly better with each other than the nonaveraged ones (cf. the black line in Fig. 6, which is duplicated from Fig. 5). In fact, the orbit-averaged spin precessing between NR and PN agrees as well as the orbital angular momentum precession, cf. Fig. 4. Thus, the difference in the spin dynamics is dominated by the nutation features, with the orbit-averaged spin dynamics agreeing well between PN and NR.

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averaged and unaveraged 2 PN precession equations, as well as the full 3.5PN precession equations and NR data. It is evident that the orbit-averaged equations do indeed reproduce the nonaveraged behavior. Further, we note that the 2PN results diverge from the NR data quickly outside of the matching region. Meanwhile the 3.5PN precession equations match the NR results much better throughout the inspiral. Therefore, to improve on the leading-order orbit-averaged precession equations, it is more important to increase the PN order than to avoid orbit-averaging.

We also test that our a posteriori orbit-averaging reproduces the analytically orbit-averaged precession equations. This is indeed the case as can be seen in Fig. 8. Shown are the angles $\angle \chi_1$ and $\angle L$ for the various choices of PN approximants. As one can see, the angle between the a posteriori-averaged PN equations and smoothed NR data (e.g. $\ddot{\chi}_1$) lies on top of the angle between the orbit-averaged PN precession equations and the smoothed NR data. Further, all of the curves lie essentially on top of one another, reflecting that a priori and apostori matching do not significantly bias the comparison. Finally, the angle between the a posteriori-averaged PN and the averaged precession equations is approximately 10–20 times smaller than the angle between PN and NR. We thus have further confidence that the ad hoc filtering procedure is a useful tool for smoothing the NR data.

To characterize the nutation features in the spin vectors, we introduce a coordinate system which is specially adapted to highlighting nutation effects. The idea is to visualize nutation with respect to the averaged spin vector $\dot{\chi}$. We compute the time-derivative $\dot{\chi}$ numerically. Assuming that the “averaged” spin is undergoing pure precession, so that $\dot{\chi} \cdot \dot{\chi} = 0$, we define a new coordinate system $(\hat{e}_1, \hat{e}_2, \hat{e}_3)$ by $\hat{e}_1 = \dot{\chi}$, $\hat{e}_2 = \dot{\chi}/|\dot{\chi}|$, $\hat{e}_3 = \hat{e}_1 \times \hat{e}_2$. The spin is now projected onto the $\hat{e}_2 - \hat{e}_3$ plane, thus showing the motion of the spin in a frame “coprecessing” with the averaged spin. This allows us to approximately decouple precession and nutation and compare them separately between PN and NR.

FIG. 6 (color online). Angle $\angle \chi_1$ between the “orbit-averaged” spins for the configuration $q^{5.0.5x}$. The non-orbit-averaged difference $\angle \chi_1$ (cf. Fig. 5) is shown for comparison. Shown is one matching interval as indicated by the thin horizontal line.

FIG. 7 (color online). Comparison of orbit averaged PN precession equations with the non-orbit-averaged equations. Plotted are $\dot{\chi}$ (left) and $\dot{L}$ (right) on the unit sphere for 2 PN averaged and nonaveraged precession equations, 3.5 PN unaveraged precession equations and NR data. The large black dot represents the centre (in time) of the matching interval (several symbols overlap here). The other black dots represent the interval $\pm 2000$ M from the matching point. The same is done for 2PN (orange dots) and 3.5PN (blue squares). Both 2PN curves lie on top of each other and match the NR data well close to the matching region but then quickly diverge away. The 3.5 PN curve matches the NR result much better throughout the inspiral.
Figure 9 plots the projection of the spins $\chi_{NR}^1$ and $\chi_{PN}^1$ onto their respective “orbit averaged” $\hat{e}_2 - \hat{e}_3$ planes. We see that the behavior of the NR spin and the PN spins are qualitatively different: For this single-spin system, the PN spin essentially changes only in the $\hat{e}_3$ direction (i.e., orthogonal to its average motion $\tilde{\chi}_{PN}$). In contrast, the NR spin undergoes elliptical motion with the excursion along its $\hat{e}_2$ axis (i.e., along the direction of the average motion) about several times larger than the oscillations along $\hat{e}_3$. The symbols plotted in Fig. 9 reveal that each of the elliptic “orbits” corresponds approximately to half an orbit of the binary, consistent with the interpretation of this motion as nutation. The features exhibited in Fig. 10 are similar across all the single-spinning precessing cases considered in this work. The small variations in spin direction exhibited in Fig. 9 are orders of magnitude smaller than parameter estimation capabilities of LIGO, e.g. [67], and so we do not expect that these nutation features will have a negative impact on GW detectors. To understand the features of Fig. 9 in more detail, it would be beneficial to carefully compare gauge conditions between NR and PN, and to consider spin supplementary conditions.

FIG. 8 (color online). Comparison of a posteriori averaging procedure described above to using orbit-averaged PN precession equations for PN evolution for configuration $q = 0.5x$. The curves labelled with $2PN_{avg}$ use orbit-averaged precession equations. A $\tilde{\chi}$ means a posteriori smoothing of $\chi$. There is virtually no difference between using the full precession equations and filtering aposteriori and using the orbit-averaged precession equations. The angle between the orbit-averaged PN results and the a posteriori-averaged PN results is 10–20 times smaller than the angles between PN and NR data showing that a posteriori-averaging does not bias the comparison. Shown is one matching interval as indicated by the thin horizontal line.

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Let us now apply our nutation analysis to the orbital angular momentum directions $\hat{l}$. Analogous to the spin, we compute averages $\tilde{\chi}_{NR}^1$ and $\tilde{\chi}_{PN}^1$, and compute the angle between the directions of the averages, $\angle L = \angle(\tilde{\chi}_{PN}, \tilde{\chi}_{NR})$. This angle—plotted in the top panel of Fig. 10—agrees very well with the difference $\angle L$ that was computed without orbit-averaging. This indicates that the nutation features of $\hat{l}$ agree between NR and PN. The top panel of Fig. 11 also plots the angle between the raw $\tilde{\chi}_{NR}$ and the averaged $\tilde{\chi}_{NR}$, i.e. the opening angle of the nutation oscillations. As is apparent in Fig. 10, the angle between $\tilde{\chi}_{NR}$ and $\tilde{\chi}_{PN}$ is about 10 times larger than the difference between NR and PN ($\angle L$ or $\angle L$), confirming that nutation features are captured. The lower panel of Fig. 10 shows the projection of $\hat{l}$ orthogonal to the direction of the average $\tilde{l}$. In contrast to the spins shown in Fig. 9, the nutation behavior of $\hat{l}$ is in close agreement between NR and PN:

FIG. 9 (color online). Comparison of a posteriori averaging procedure described above to using orbit-averaged PN precession equations for PN evolution for configuration $q = 0.5x$. The curves labelled with $2PN_{avg}$ use orbit-averaged precession equations. A $\tilde{\chi}$ means a posteriori smoothing of $\chi$. There is virtually no difference between using the full precession equations and filtering aposteriori and using the orbit-averaged precession equations. The angle between the orbit-averaged PN results and the a posteriori-averaged PN results is 10–20 times smaller than the angles between PN and NR data showing that a posteriori-averaging does not bias the comparison. Shown is one matching interval as indicated by the thin horizontal line.

FIG. 9 (color online). The projection of $\chi_{NR}^1$ and $\chi_{PN}^1$ onto the $\hat{e}_2 - \hat{e}_3$ plane described in the text for case $q = 0.5x$. The system is shown in the interval $t - t_{merge} \in [-6662, -1556]/c_{138}$. Meanwhile, the NR data show variations in $\hat{e}_2$ and $\hat{e}_3$ directions of comparable magnitude. The solid symbols (black diamond for NR, red square for PN) indicate the data at the start of the plotted interval, chosen such that $\chi_1 \cdot \tilde{n}$ is maximal—i.e., where the spin projection into the orbital plane is parallel to $\tilde{n}$. The subsequent four open symbols (blue diamonds for NR, green squares for PN) indicating the position $1/8$-th, $1/4$-th, $3/8$-th and $1/2$ of an orbit later.
We now extend our precession dynamics analysis to the remaining five primary precessing NR simulations listed in Table I. The top left panel of Figure 11 shows $\angle L$. The difference in the direction of the normal to the orbital plane is small; generally $\angle L \lesssim 10^{-2}$ radians, except close to merger. Thus it is evident that the trends seen in Fig. 4 for $\angle L$ hold across all the precessing cases. To make this behavior clearer, we parameterize the inspiral using the orbital phase instead of time, by plotting the angles versus the orbital phase in the NR simulation, as shown in the top right panel of Fig. 11. Thus, until a few orbits to merger PN represents the precession and nutation of the orbital plane well.

The bottom left panel of Fig. 11 establishes qualitatively good agreement for $\angle \hat{\chi}_1$, with slightly higher values than $\angle L$. As already illustrated in Fig. 6, nutation features dominate the difference. Averaging away the nutation features, we plot the angle $\angle \hat{\chi}_1$ between the smoothed spins in the bottom left panel of Fig. 11, where the behavior of $\angle \hat{\chi}_1$ is very similar to that of $\angle L$. This confirms that the main disagreement between PN and NR spin dynamics comes from nutation features, and suggests that the secular precession of the spins is well captured across all cases, whereas the nutation of the spins is not. For completeness, we also show a parametric plot of $\angle L$ and $\angle S$ versus orbital frequency in the NR simulation in Fig. 12.

All configurations considered so far except q1.97_random have $\vec{S} \cdot \hat{\ell} = 0$ at the start of the simulations, where $\vec{S} = \vec{S}_1 + \vec{S}_2$ is the total spin angular momentum of the system. When $\vec{S} \cdot \hat{\ell} = 0$, several terms in PN equations vanish, in particular the spin orbit terms in the expansions of the binding energy, the flux and the orbital precession frequency, see Eqs. (A14), (A15), and (A31) in Appendix A.

To verify whether $\vec{S} \cdot \hat{\ell} = 0$ introduces a bias to our analysis, we perform our comparison on an additional set of 31 binaries with randomly oriented spins. These binaries have mass ratio $1 \leq q \leq 2$, spin magnitudes $0 \leq \chi_{1,2} \leq 0.5$, and correspond to cases SXS:BBH:0115—SXS:BBH:0146 in the SXS catalog. Fig. 13 plots $\angle L$ for these additional 31 PN-NR comparisons in gray, with q1.97_random highlighted in orange. The disagreement between PN and NR is similarly small in all of these cases, leading us to conclude that our results are robust in this region of the parameter space.

For both, $\hat{\ell}$ precesses in a circle around $\hat{\ell}$, with identical period, phasing, and with almost identical amplitude. We also point out that the shape of the nutation features differs between $\hat{\ell}$ and $\hat{\chi}_1$: $\hat{\ell}$ circles twice per orbit around its average $\bar{\hat{\ell}}$, on an almost perfect circle with equal amplitude in the $\hat{\ell}_2 - \hat{\ell}_3$ direction.

We now extend our precession dynamics analysis to the orbital phase comparisons

Along with the precession quantities described above, the orbital phase plays a key role in constructing PN waveforms. We use $\Phi_{\Delta}$, a geometrically invariant angle that reduces to the orbital phase difference for nonprecessing binaries (cf. Sec. II C) to characterize phasing effects. We focus on single spin systems with mass ratios from 1 to 8, where the more massive black hole carries a spin of $\chi_1 = 0.5$, and where the spin is aligned or antialigned with the orbital angular momentum, or where the spin is initially tangent to the orbital plane. We match all NR simulations to post-Newtonian inspiral dynamics as described in Sec. II D, using the 12 matching intervals specified in Eqs. (19) and (20). We then compute the phase difference $\Phi_{\Delta}$ at the time

FIG. 10 (color online). Characterization of nutation effects of the orbital angular momentum. Top: angle $\angle L$ between the “averaged” $\hat{\ell}$ in PN and NR for the configuration q5_0.5x (thick red line). $\angle L$ is shown in thin black line for comparison (cf. Fig. 6). The thin blue line shows $\angle(\hat{\ell}, \hat{\ell})$ between the averaged and the filtered signal. Note that it is larger than both $\angle L$ and $\angle \hat{L}$. Bottom: the projection of $\hat{L}^{\text{NR}}$ (gray) and $\hat{L}^{\text{PN}}$ (red) onto the $\hat{\ell}_2 - \hat{\ell}_3$ plane described in the text for case q5_0.5x (cf. Fig. 10). The system is shown in the interval $[-6662, -1556]$. Both PN and NR show the same behavior, in contrast to the behavior of the spin in Fig. 9. The PN-NR matching interval is indicated by the horizontal line in the top panel.
at which the NR simulation reaches orbital frequency $m\Omega_{\text{NR}} = 0.03$.

The results are presented in Fig. 14, grouped based on the initial orientation of the spins: aligned, antialigned, and in the initial orbital plane. For aligned runs, there are clear trends for Taylor T1 and T5 approximants: for T1, differences decrease with increasing mass ratio (at least up to $q = 8$); for T5, differences increase. For Taylor T4, the

FIG. 11 (color online). Comparison of orbital plane and spin precession for the primary six precessing NR simulations. Top Left: $\angle L$ as a function of time to merger. Top right: $\angle L$ as a function of orbital phase in NR. Bottom left: $\angle \chi_1$ as a function of orbital phase. Bottom right: $\angle \tilde{\chi}_1$ between the averaged spins. All data plotted are averages over 12 matching intervals, cf. Fig. 3, utilizing the Taylor T4 PN approximant. The thin horizontal lines in the top left panel show the widest edges of the PN matching intervals.

FIG. 12 (color online). Comparison of orbital plane and spin precession for the primary six precessing NR simulations as functions of orbital frequency in NR. Right: $\angle L$; Left: $\angle \chi_1$. All data plotted are averages over 12 matching intervals, cf. Fig. 3, utilizing the Taylor T4 PN approximant.
phase difference $\Phi_\Delta$ has a minimum and there is an overall increase for higher mass ratios. For antialigned runs, Taylor T5 shows the same trends as for the aligned spins. Taylor T4 and T1 behaviors, however, have reversed: T4 demonstrates a clear increasing trend with mass ratio, whereas T1 passes through a minimum with overall increases for higher mass ratios. Our results are also qualitatively consistent with the results described in [13] as we find that for equal mass binaries, the Taylor T4 approximant performs better than the Taylor T1 approximant (both for aligned and antialigned spins).

For the in-plane precessing runs, we see clear trends for all 3 approximants: Taylor T4 and T5 both show increasing differences with increasing mass ratio, and T1 shows decreasing differences. These trends for precessing binaries are consistent with previous work on nonspinning binaries [17], which is expected since for $S \cdot \hat{\ell}$ many of the same terms in the binding energy and flux vanish as for nonspinning binaries. Overall, we find that for different orientations and mass ratios, no one Taylor approximant performs better than the rest, as expected if the differences between the approximants arise from different treatment of higher-order terms.

C. Convergence with PN order

So far all comparisons were performed using all available post-Newtonian information. It is also instructive to consider behavior at different PN order, as this reveals the convergence properties of the PN series, and allows estimates of how accurate higher order PN expressions might be.

The precession frequency $\varpi$, given in Eq. (A31), is a product of series in the frequency parameter $x$. We multiply out this product, and truncate it at various PN orders from leading order (corresponding to 1.5PN) through next-to-next-to-leading order (corresponding to 3.5PN). Similarly, the spin precession frequencies $\tilde{\Omega}_{1,2}$ in Eqs. (2) and (A32) are power series in $x$. We truncate the power series for $\tilde{\Omega}_{1,2}$ in the same fashion as the power series for $\varpi$, but keep the orbital phase evolution at 3.5PN order, where we use the TaylorT4 prescription to implement the energy flux balance. For different precession-truncation orders, we match the PN dynamics to the NR simulations with the same techniques and at the same matching frequencies as in the preceding sections.

When applied to the NR simulation $q_{3,0.5}$, we obtain the results shown in Fig. 15. This figure shows clearly that with increasing PN order in the precession equations, PN precession dynamics tracks the NR simulation more and more accurately. When only the leading order terms of the precession equations are included (1.5PN order), $\angle L$ and $\angle \chi_1$ are $\approx 0.1$ rad; at 3.5PN order this difference drops by nearly two orders of magnitude.

We repeat this comparison for our six main precessing cases from Table I. The results are shown in Fig. 16 and once again the angles are evaluated at the time the NR simulation reaches orbital frequency of $m\Omega_{NR} = 0.03$. It is evident that for all cases $\angle L$ decreases with increasing order in the precession equations with almost 2 orders of magnitude improvement between leading order and
next-to-next leading order truncations. A similar trend is seen in the convergence of the spin angle $\angle \chi_1$ shown in the bottom panel of Fig. 16. The angle decreases with PN order almost monotonically for all cases except $q_{1.0 \_twospins}$. However, this is an artificial consequence of picking a particular matching point at $m \Omega_{NR} = 0.03$: as can be seen from the bottom panel of Fig. 15, $\angle \chi_1$ shows large oscillations and it is a coincidence that the matching point happens to be in a "trough" of $\chi_1$.

So far we have varied the PN order of the precession equations, while keeping the orbital frequency evolution at 3.5PN order. Let us now investigate the opposite case: varying the PN order of the orbital frequency and monitoring its impact on the orbital phase evolution. We keep the PN order of the precession equations at 3.5PN, and match PN with different orders of the orbital frequency evolution (and TaylorT4 energy-balance prescription) to the NR simulations. We then evaluate $\Phi_\Delta$ (a quantity that reduces to the orbital phase difference in cases where the latter is unambiguously defined) at the time at which the NR simulation reaches the frequency $m \Omega_{NR} = 0.03$. We examine our six primary precessing runs, and also the aligned-spin and antialigned spin binaries listed in Table I.

When the spin is initially in the orbital plane, as seen in the top panel of Fig. 17, the overall trend is a nonmonotonic error decrease with PN order, with spikes at 1 and 2.5 PN orders as has been seen previously with nonspinning binaries [11]. All of the aligned cases show a large improvement at 1.5 PN order, associated with the leading order spin-orbit contribution. The phase differences then spike at 2 and 2.5 PN orders and then decrease at 3 PN order. Finally, different cases show different results at 3.5 PN with some showing decreases differences while for others the differences increase.

For the antialigned cases the picture is similar to precessing cases with a spike at 1 and 2.5 PN orders and monotonic improvement thereafter. The main difference from precessing cases is the magnitude of the phase differences, which is larger by a factor of $\sim 5$ at 3.5 PN order for the antialigned cases (see for example $q_{1.5\_s0.5x\_0}$).

These results suggest that convergence of the orbital phase evolution depends sensitively on the exact
parameters of the system under study. Further investigation of the parameter space is warranted.

D. Impact of PN spin truncation

As mentioned in Sec. II A 2, post-Newtonian expansions are not fully known to the same orders for spin and nonspin terms. Thus, for example, the expression for flux $\mathcal{F}$ is complete to 3.5 PN order for nonspinning systems, but spinning systems may involve unknown terms at 2.5 PN order; a similar statement holds for $dE/dx$. This means that when the ratio in Eq. (4), $\mathcal{F}/(dE/dx)$, is reexpanded as in the T4 approximant, known terms will mix with unknown terms. It is not clear, a priori, how such terms should be handled when truncating that reexpanded series.

Here we examine the effects of different truncation strategies. We focus on the Taylor T4 approximant while considering various possible truncations of the reexpanded form of $\mathcal{F}/(dE/dx)$. We denote these possibilities by the orders of (1) the truncation of nonspin terms, (2) the truncation of spin-linear terms, and (3) the truncation of spin-quadratic terms. Thus, for example, in the case where we keep nonspin terms to 3.5 PN order, keep spin-linear terms to 2.5 PN order, and keep spin-quadratic terms only to 2.0 PN order, we write (3.5, 2.5, 2.0). We consider the following five possibilities:

(i) (3.5, 3.5, 3.5)
(ii) (3.5, 4.0, 4.0)
(iii) (3.5, 2.5, 2.0)
(iv) (3.5, 3.5, 2.0)
(v) (3.5, 4.0, 2.0).

To increase the impact of the spin-orbit terms, we examine aligned and antialigned cases from Table I, with results presented in Fig. 18, where once more $\Phi_\Delta$ is evaluated at the time at which the NR simulation reaches the frequency $m\Omega_{NR} = 0.03$. For aligned cases, no one choice of spin truncation results in small differences across all mass ratios. All choices of spin truncation excepting (3.5, 4.0, 4.0) have increasing errors with increasing mass ratio.
ratio. Truncating spin corrections at 2.5 PN order (3.5, 2.5, 2) consistently results in the worst matches. On the other hand, we find that, for antialigned runs, adding higher order terms always improves the match, keeping all terms yields the best result, and all choices of truncation give errors which are monotonically increasing with mass ratio. Overall, antialigned cases have larger values of $\Phi_\Delta$ when compared to cases with same mass ratios. This result is consistent with findings by Nitz et al. [23] for comparisons between TaylorT4 and EOBNRv1 approximants.

E. Further numerical considerations

1. Numerical truncation error

Still to be addressed is the effect of the resolution of NR simulations in the present work. The simulation q1_twospins is available at four different resolutions labeled N1, N2, N3 and N4. We match each of these four numerical resolutions with the Taylor T4 approximant, and plot the resulting phase differences $\Phi_\Delta$ in Fig. 19 as the data with symbols and error bars (recall that the error bars are obtained from the 12 different matching regions we use, cf. Fig. 3). All four numerical resolutions yield essentially the same $\Phi_\Delta$. We furthermore match the three lowest numerical resolutions against the highest numerical resolution N4 and compute the phase difference $\Phi_\Delta$. The top panel of Figure 19 shows $\Phi_\Delta$ computed with these 4 different numerical resolutions. All the curves lie on top of each other and the differences between them are well within the uncertainties due to the matching procedure. The bottom panel shows the differences in $\Phi_\Delta$ between the highest resolution and all others. Throughout most of the inspiral, the difference is $\sim 10\%$. Similar behavior is observed in other cases where multiple resolutions of NR simulations are available. We therefore conclude that the effects of varying numerical resolution do not impact our analysis.

2. Numerical gauge change

The simulation SXS:BBH:0058 in the SXS catalog uses identical BBH parameters than q5_0.5x, but suffers from two deficiencies, exploration of which will provide some additional insights. First, the switch from generalized harmonic gauge with fixed gauge-source functions [11] to dynamical gauge-source functions [54,55] happens near the middle of the inspiral, rather than close to merger as for the other simulations considered. This will give us an opportunity to investigate the impact of such a gauge change, the topic of this subsection. Second, this simulation also used too low resolution in the computation of the black hole spin during the inspiral, which we will discuss in the next subsection. We emphasize that the comparisons presented above did not utilize SXS:BBH:0058, but rather a rerun with improved technology. We use SXS:BBH:0058 in this section to explore the effects of its deficiencies.

While the difference between PN and NR gauges does not strongly impact the nature of the matching results, a gauge change performed during some of the runs does result in unphysical behavior of physical quantities such as the orbital frequency. Figure 20 demonstrates this for case q5_s0.5x. The old run SXS:BBH:0058 with the gauge change exhibits a bump in the orbital frequency (top panel), which is not present in the rerun (solid curve). When matching both the old and the new run to PN, and computing the phase difference $\Phi_\Delta$, the old run exhibits a nearly discontinuous change in $\Phi_\Delta$ (bottom panel, dashed curves) while no such discontinuity is apparent in the rerun.

3. Problems in quasilocal quantities

Computation of the quasilocal spin involves the solution of an eigenvalue problem on the apparent horizon followed by an integration over the apparent horizon, cf. [68–70]. In the simulations q1.0_0.5x, q1.5_0.5x and q3.0_0.5x and in SXS:BBH:0058 (corresponding to q5.0_5x), too low...
numerical resolution was used for these two steps. While the evolution itself is acceptable, the extracted spin shows unphysical features. Most importantly, the reported spin magnitude is not constant, but varies by several per cent. Figure 21 shows as example $\chi$ from SXS:BBH:0058. For $t - t_{\text{merge}} \leq 3200M$ oscillations are clearly visible. These oscillations vanish at $t - t_{\text{merge}} \approx 3200M$, coincident with a switch to damped harmonic gauge (cf. Sec. III E 2). Similar oscillations in $q_3_{0.5}$ disappear when the resolution of the spin computation is manually increased about $1/3$ through the inspiral, without changing the evolution gauge. Our new rerun $q_{5}_{0.5x}$ (using damped harmonic gauge throughout), also reports a clean $\chi$ (cf. Fig. 21). Thus, we conclude that the unphysical variations in the spin magnitude are only present if both the resolution of the spin computation is low, and the old gauge conditions of constant $H_a$ are employed.

The NR spin magnitude is used to initialize the PN spin magnitude [cf. Eq. (14)]. Therefore, an error in the calculation of the NR spin would compromise our comparison with PN. For the affected runs, we correct the spin reported by the quasilocal spin computation by first finding all maxima of the spin-magnitude $\chi$ between $500M$ and $2000M$ after the start of the numerical simulation. We then take the average value of $\chi$ at those maxima as the corrected spin-magnitude of the NR simulation. Figure 21 shows the case $q_{5}_{0.5x}$ as well as the rerun described in Sec. III E 2. It is evident that this procedure produces a spin value which is very close to the spin in the rerun where the problematic behavior is no longer present. Thus, we adopt it for the

FIG. 20 (color online). Gauge change during numerical simulation $q_{5}_{0.5x}$. The solid curves represent the recent rerun of $q_{5}_{0.5x}$ that is analyzed in the rest of this paper. The dashed curves represent an earlier run SXS:BBH:0058 which changes the gauge at $t - t_{\text{merge}} \approx -3200M$. Top: behavior of the orbital frequency $m\Omega$ in evolution with (dashed curve) and without gauge change (solid curve). Bottom: $\Phi_\Delta$ for all Taylor approximants. To avoid matching during the gauge change, the matching was done with $m\Omega_c = 0.017$.

FIG. 21 (color online). Top: The magnitude of the spin as a function of time in the original run (black) and the new run (blue) as well as the value computed with the procedure described in the text (orange). Middle panel: angles between the spins and normals to the orbital plane (thin curves) and their averaged values (bold curves) for the original run and the rerun. Lower panel: $\angle \tilde{\chi}$ and $\angle \tilde{\ell}$ for both the old run and the rerun (the data of this panel are averaged over 12 matching intervals, cf. Fig. 3). To avoid matching during the gauge change, the matching was done with $m\Omega_c = 0.017$. 
three cases where an oscillation in the spin magnitude is present.

The nutation features shown in Fig. 9 are qualitatively similar for all our simulations, independent of resolution of the spin computation and evolution gauge. When the spin is inaccurately measured, the nutation trajectory picks up extra modulations, which are small on the scale of Fig. 9 and do not alter the qualitative behavior.

The lower two panels of Fig. 21 quantify the impact of inaccurate spin measurement on the precession-dynamics comparisons performed in this paper: The middle panel shows the differences between the spin directions in the original 0058 run and our rerun q5_0.5x. The spin directions differ by as much as 0.01 radians. However, as the lower panel shows, this difference can mostly be absorbed by the PN matching, so that $\angle L_1$ and $\angle L$ are of similar magnitude of about $10^{-3}$ radians.

IV. DISCUSSION

We have presented an algorithm for matching PN precession dynamics to NR simulations which uses constrained minimization. Using this algorithm, we perform a systematic comparison between PN and NR for precessing binary black hole systems. The focus of the comparison is black hole dynamics only, and we defer discussion of waveforms to future work. By employing our matching procedure, we find excellent agreement between PN and NR for the precession and nutation of the orbital plane. The NR spin direction $\hat{\chi}$ generally lies within $10^{-2}$ radians (cf. Fig. 11). Moreover, nutation features on the orbital time scale also agree well between NR and PN (cf. Fig. 10).

For the black hole spin direction, the results are less uniform. The NR spin direction $\hat{\chi}^{\text{NR}}$ shows nutation features that are qualitatively different than the PN nutation features (cf. Fig. 9). The disagreement in nutation dominates the agreement of $\hat{\chi}_1^{\text{NR}}$ with $\hat{\chi}_1^{\text{PN}}$; averaging away the nutation features substantially improves agreement (cf. Fig. 6). The orbit-averaged spin directions agree with PN to the same extent that the $\hat{\chi}$ direction does (with and without orbit averaging) (cf. Fig. 11).

Turning to the convergence properties of PN, we have performed PN-NR comparisons at different PN order of the precession equations. For both orbital angular momentum $\hat{\chi}$ and the spin direction $\hat{\chi}_1$, we observe that the convergence of the PN results toward NR is fast and nearly universally monotonic (cf. Fig. 16). At the highest PN orders, the spin results might be dominated by the difference in nutation features between PN and NR.

The good agreement between PN and NR precession dynamics are promising news for gravitational wave modeling. Precessing waveform models often rely on the post-Newtonian precession equations, e.g. [24,71]. Our results indicate that the PN precession equations are well suited to model the precessing frame, thus reducing the problem of modeling precessing waveforms to the modeling of orbital phasing only.

The accuracy of the PN orbital phase evolution, unfortunately, does not improve for precessing systems. Rather, orbital phasing errors are comparable between nonprecessing and precessing configurations (cf. Fig. 17). Moreover, depending on mass-ratio and spins, some Taylor approximants match the NR data particularly well, whereas others give substantially larger phase differences (cf. Fig. 14). This confirms previous work [14,17,20,31,72] that the PN truncation error of the phase evolution is important for waveform modeling.

We have also examined the effects of including partially known spin contributions to the evolution of the orbital frequency for the Taylor T4 approximant. For aligned runs, including such incomplete information usually improves the match, but the results are still sensitive to the mass ratio of the binary (top panel of Fig 18). For antialigned runs, it appears that incomplete information always improves the agreement of the phasing between PN and NR (bottom panel of Fig 18).

In this work we compare gauge-dependent quantities, and thus must examine the impact of gauge choices on the conclusions listed above. We consider it likely that the different nutation features of $\hat{\chi}_1$ are determined by different gauge choices. We have also seen that different NR gauges lead to measurably different evolutions of $\hat{\chi}$, $\hat{\epsilon}$, and the phasing (cf. Figs. 20 and 21). We expect, however, that our conclusions are fairly robust to the gauge ambiguities for two reasons. First, in the matched PN-NR comparison, the impact of gauge differences is quite small (cf. lowest panel of Fig. 21). Second, the near universal, monotonic, and quick convergence of the precession dynamics with precession PN order visible in Fig. 16 would not be realized if the comparison were dominated by gauge effects. Instead, we would expect PN to converge to a solution different from the NR data.

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Meanwhile for the flux $\mathcal{F}$:

$$b_2 = \frac{1247}{336} - \frac{35}{12} \nu, \quad \text{(A22)}$$

$$b_3 = 4\pi - 4s_I - \frac{5}{4} \delta \sigma_I, \quad \text{(A23)}$$
where \( \gamma_E \) denotes Euler’s constant.

### a. Precession dynamics

The evolution of the orbital plane is governed by the frequency \( \tilde{\sigma} \) in Eq. (1a), which is defined in terms of two auxiliary quantities, \( \gamma = m/r \) and \( a_i = \vec{\alpha} \cdot \hat{e} \):

\[
\gamma = x \left\{ 1 + \frac{3 - \nu}{3} - x + \frac{3a_1 + 5s_1}{3} x^{3/2} + \frac{12 - 65 \nu}{12} x^2 + \left( \frac{30 + 8 \nu}{9} - s_1 - 2 \sigma \right) x^{5/2} \right. \\
\left. + \left[ 1 + \nu \left( \frac{2203}{250} - \frac{41 \pi^2}{192} + \frac{229 \nu^2}{36} + \frac{\nu^3}{81} \right) x^3 + \left( \frac{60 - 12 \nu - 72 \nu^2}{12} s_1 + \frac{16 - 61 \nu - 16}{6} \sigma \right) x^{7/2} + x^2 (\tilde{s}_0 - 3 (\tilde{s}_0 \cdot \tilde{e})^2) \right] \right\},
\]

(A29)

\[
a_i = \frac{x^2}{m} \left\{ 7s_n + 3 \sigma \delta + x \left[ s_n \left( -\frac{29 \nu}{3} - 10 \right) + \sigma \left( \frac{9 \nu}{2} - 6 \right) \right] \right. \\
\left. + x^2 \left[ s_n \left( \frac{52 \nu^2}{9} + \frac{59 \nu}{4} + \frac{3}{2} \right) + \sigma \delta \left( \frac{17 \nu^2}{6} + \frac{73 \nu}{8} + \frac{3}{2} \right) \right] \right\} - \frac{3x^4}{m} (\tilde{s}_0 \cdot \tilde{e}) (\tilde{s}_0 \cdot \hat{n}).
\]

(A30)

Note that we have dropped the pure gauge term \(-\frac{2\nu}{3} \ln (r/r_0)\) from \( \gamma \). We now have

\[
\tilde{\sigma} = \frac{a_i \gamma}{x^{3/2}}.
\]

(A31)

The spins obey Eqs. (2) with

\[
\tilde{\Omega}_i = \frac{x^4}{m} \left\{ -\frac{3 \delta + 2 \nu + 3}{4} + x \left[ \frac{10 \nu - 9}{16} \delta - \frac{\nu^2}{24} + \frac{5 \nu}{4} + \frac{9}{16} \right] + x^2 \left[ -\frac{5 \nu^2 + 15 \nu^2 - 27}{32} \delta - \frac{\nu^3}{48} - \frac{105 \nu^2}{32} + \frac{3 \nu}{16} + \frac{27}{32} \right] \right\} \\
+ \frac{x^3}{m} \left[ \frac{3m^2}{q} (\tilde{\chi}_1 \cdot \hat{n}) \hat{n} - m^2 \tilde{\chi}_2 + 3m^2_2 (\tilde{\chi}_2 \cdot \hat{n}) \hat{n} \right].
\]

(A32)
Comparing Post-Newtonian and Numerical ...
need to rotate \( \mathbf{\hat{x}}' \) onto \( \mathbf{\hat{n}} \), while leaving \( \mathbf{\hat{\ell}} \) in place. Of course, the \( \mathbf{\hat{n}}-\mathbf{\hat{x}}' \) is orthogonal to \( \mathbf{\hat{\ell}} \), so we just perform a rotation in that plane. This is easily accomplished by the following formula:

\[
R_t = \sqrt{-\mathbf{\hat{n}}(\mathbf{\hat{R}}_t \mathbf{\hat{x}}')R_t},
\]

Again, the square roots are to be evaluated using Eq. (B6).

3. Comparing frame rotors

Reference [60] introduced a simple, geometrically invariant measure \( R_\Phi \) that encodes the difference between two precessing systems as a function of time, easily reduced to a single real number \( \Phi_\Delta \) expressing the magnitude of that difference. These quantities were mentioned in Sec. II C without much motivation; here we briefly review that motivation.

In general, we assume that there are two (analytical or numerical) descriptions of the same physical system, and that we have two corresponding frames \( R_{\hat{I}A} \) and \( R_{\hat{I}B} \). To understand the difference between the frames, we can simply take the rotation that takes one frame onto the other. In this case, the rotor taking frame A onto frame B is

\[
R_\Delta := R_{\hat{I}B} R_{\hat{I}A}.
\]

Rotors compose by left multiplication, so it is not hard to see that this does indeed take \( R_{\hat{I}A} \) onto \( R_{\hat{I}B} \) because the inverse of \( R_{\hat{I}A} \) is just its conjugate, so \( R_\Delta R_{\hat{I}A} = R_{\hat{I}B} \).

A particularly nice feature of \( R_\Delta \) is that it is completely independent of the inertial basis frame (\( \mathbf{\hat{x}}, \mathbf{\hat{y}}, \mathbf{\hat{z}} \)) with respect to which we define the moving frames. That is, if we have another basis frame (\( \mathbf{\hat{x}}', \mathbf{\hat{y}}', \mathbf{\hat{z}}' \)), there is some \( R_\delta \) such that \( \mathbf{\hat{x}}' = R_\delta \mathbf{\hat{x}} \), etc. The frame rotors would transform as \( R_{\hat{I}A} \rightarrow R'_{\hat{I}A} = R_{\hat{I}A} R_\delta \), in which case we obtain

\[
R_{\hat{I}B}' R'_{\hat{I}A} = R_{\hat{I}B} R_\delta R_{\hat{I}A} = R_{\hat{I}B} R_{\hat{I}A}.
\]

That is, \( R_\Delta \) is invariant.

Now, we seek a relevant measure of the magnitude of the rotation \( R_\Delta \). We know that it may be written as a rotation through an angle \( \phi \) about an axis \( \mathbf{\hat{v}} \). Clearly, \( \phi \) is the measure we seek. The rotor corresponding to such a rotation is given by \( R = \exp[\phi \mathbf{\hat{v}}/2] \). Thus, to find the angle, we just use the logarithm: \( \phi = 2 \log |R| \), where the norm is the usual vector norm. Again, the formula for the logarithm of a rotor is a simple combination of standard trigonometric functions applied to real numbers, as shown above. Using this interpretation with our difference rotor, we see that the appropriate definition is
The last equation becomes

\[ \Phi(R_A) = \Phi(A) \text{ and } \Phi(R_B) = \Phi(B). \]

The domain of this function is a rotation group, which could be the one-dimensional group U(1) for nonprecessing systems, but must be the full three-dimensional group SU(2) for general precessing systems. The range of \( \Phi \) is the usual range of phases, the additive group of real numbers modulo \( 2\pi \). It will be useful to note that this is isomorphic to U(1).

Finally, nondegeneracy is the condition that \( \Phi_A - \Phi_B = 0 \) [or equivalently \( \Phi(R_A) = \Phi(R_B) \)] if and only if \( R_A = \pm R_B \).

The condition of geometric invariance can be written as a condition on \( \Phi \) itself. If, for example, we measure everything with respect to some basis \( (\hat{x}, \hat{y}, \hat{z}) \), and then measure again with respect to some other basis \( (\hat{x}', \hat{y}', \hat{z}') \), we should get the same answer. Now, there is some rotor \( R_A \) that takes the first basis into the second. If \( R_A \) is defined with respect to the first basis, then the equivalent quantity will be \( R_A R_B \) with respect to the second. Geometric invariance is then the statement

\[ \Phi(R_A R_B) - \Phi(R_B R_A) = \Phi(R_A) - \Phi(R_B), \]

for any choice of \( R_B \) in SU(2). We will show that there is no such \( \Phi \) because the rotation group SU(2) is not isomorphic to U(1).

Since Eq. (B12) is true for any rotor \( R_B \), we can choose \( R_B = R_B^{-1} \), and find that

\[ \Phi(R_A R_B^{-1}) - \Phi(1) = \Phi(R_A) - \Phi(R_B). \]

Now, we define another function \( \Phi'(R) = \Phi(R) - \Phi(1) \). The last equation becomes

\[ \Phi'(R_A R_B^{-1}) = \Phi'(R_A) - \Phi'(R_B). \]

In exactly the same way, we can see that

\[ \Phi'(R_B R_A^{-1}) = \Phi'(R_B) - \Phi'(R_A) = -\Phi'(R_A R_B^{-1}). \]

This must be true for all values of \( R_A \) and \( R_B \), so we have shown that

\[ \Phi'(R^{-1}) = -\Phi'(R) \]

for arbitrary \( R \). Therefore, we can also see from Eq. (B14) that

\[ \Phi'(R_1 R_2) = \Phi'(R_1) + \Phi'(R_2) \]

for arbitrary \( R_1 \) and \( R_2 \). This is precisely the statement that \( \Phi' \) is a group homomorphism [from SU(2) to the additive group of real numbers modulo \( 2\pi \)].

However, now we can impose the condition that \( \Phi_A - \Phi_B = 0 \) if and only if \( R_A = \pm R_B \). Using the properties of homomorphism, it is clear that this is equivalent to the statement that the set of all elements that map to 0 under \( \Phi' \) (the kernel) is just ker \( \Phi' = \{-1, 1\} \).

Then, the first group isomorphism theorem [76] says that the image of \( \Phi' \) is isomorphic to SU(2) modulo this kernel, which of course is just SO(3). But the image of \( \Phi' \) is (possibly a subgroup of) the group U(1), which is obviously not isomorphic to SO(3). Therefore, it is impossible to construct a function \( \Phi \) fulfilling our requirements for precessing systems.

This conclusion holds whenever \( R_A \) and \( R_B \) come from a noncommutative group. Topological structures associated with SU(2), SO(3), and U(1) are completely unused in this proof. However, if we now consider the standard topology of SO(3), we know that it is possible to find noncommuting elements inside any neighborhood of any point—and in particular, inside any neighborhood of the identity. But precessing systems will necessarily explore some such neighborhood, which means that their orientations may be described by noncommuting rotors \( R_A \) and \( R_B \). Thus, \( \Phi_A - \Phi_B \) would be an inadequate measure of rotations for any system with any nonzero amount of precession.

It is, however, interesting to note that if we could restrict our rotations (including the allowed coordinate rotations \( R_B \)) to some subgroup of SU(2) isomorphic to U(1), there would be no contradiction. This is why it is possible to construct a useful measure of the form \( \Phi_A - \Phi_B \) for nonprecessing systems—because the rotations can be restricted to rotations about the orbital axis, which results in precisely the group U(1). On the other hand, for precessing systems, the measure \( \Phi_A \) described in Secs. II C and B 3 is able to satisfy both key features of a useful measure (nondegeneracy and geometric invariance) because it simply does not attempt to define a homomorphism from the rotation group; rather, it defines a (nonhomomorphic, but nondegenerate and rotationally invariant) function from two copies of the rotation group onto the phase group, SU(2) × SU(2) → U(1).

---

7 Even though it is a double cover of the physical rotation group SO(3), we use SU(2) here for consistency of notation, because it is the group of unit quaternions. The proof would actually be slightly simpler for SO(3); we would have \( \Phi(R_A) = \Phi(R_B) \), if and only if \( R_A = R_B \), and ker \( \Phi' = \{1\} \).

8 Note that this means only that \( \Phi' \) is a group homomorphism, rather than a topological group homomorphism; \( \Phi' \) (equivalently \( \Phi \)) is not required to be continuous.


