DYNAMICAL INVARIANTS FOR GENERAL RELATIVISTIC TWO-BODY SYSTEMS AT THE THIRD POST-NEWTONIAN APPROXIMATION

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Dynamical invariants for general relativistic two-body systems at the third post-Newtonian approximation

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We extract all the invariants (i.e. all the functions which do not depend on the choice of phase-space coordinates) of the dynamics of two point-masses, at the third post-Newtonian (3PN) approximation of general relativity. We start by showing how a contact transformation can be used to reduce the 3PN higher-order Hamiltonian derived by Jaranowski and Schäfer [2] to an ordinary Hamiltonian. The dynamical invariants for general orbits (considered in the center-of-mass frame) are then extracted by computing the radial action variable $\oint p_r dr$ as a function of energy and angular momentum. The important case of circular orbits is given special consideration. We discuss in detail the plausible ranges of values of the two quantities $\omega_{\rm static}$, $\omega_{\rm kinetic}$ which parametrize the existence of ambiguities in the regularization of some of the divergent integrals making up the Hamiltonian. The physical applications of the invariant functions derived here (e.g. to the determination of the location of the last stable circular orbit) are left to subsequent work.

I. INTRODUCTION

Binary sytems made of compact objects (neutron stars or black holes) are the most promising candidate sources for ground based interferometric gravitational-wave detectors such as LIGO and VIRGO. In the case of (stellar) black holes the gravitational waveform will enter the detector bandwidth only at the last stage of the inspiral motion, just before the inspiral turns into a plunge. The detection of these gravitational signals will be possible only by correlating the detector output with sufficiently accurate copies of the expected signals ("matched filtering"). It is therefore very important to have the best possible analytical control of the dynamics of general relativistic two-body systems. The equations of motion of binary systems have been derived some years ago at the 5/2 post-Newtonian (2.5PN) approximation[1] [1]. Recently, it has been possible to derive the third post-Newtonian (3PN) dynamics of point-mass systems [2], though with some remaining ambiguity due to the need to regularize the divergent integrals caused by the use of Dirac-delta-function sources. The knowledge of the conservative part of the dynamics of binary systems must then be completed by a correspondingly accurate knowledge of the gravitational-wave luminosity (used, heuristically, to derive an accurate estimate of the radiation damping effects which drive the inspiral motion of binary systems). The gravitational-wave luminosity is currently known to the *fractional* 2.5PN accuracy [3]. By combining the 2PN-level conservative dynamics [1] with the 2.5PN gravitational-wave luminosity [3] one has recently constructed some (improved) filters (P-approximants) [4], for application to gravitational-wave data analysis problems.

The main purpose of this work is to extract all the *invariants*, i.e., the functions which do not depend on the choice of coordinates (in space or phase-space), of the 3PN dynamics derived in Ref. [2]. This task is important for three reasons: (i) some of the invariant functions are directly useful for deriving the 3PN "phasing formula" of inspiralling binaries, i.e., for constructing 3PN-accurate gravitational-wave filters; (ii) we shall use, in a companion paper [5], some of the invariants derived below to determine the location of the Last (circular) Stable Orbit which marks the transition between the inspiral and the plunge, and (iii) from a practical point of view, the dynamical invariants will be quite useful for comparing the 3PN ADM Hamiltonian dynamics of [2] with forthcoming derivations of the 3PN equations of motion in harmonic coordinate systems [6].

[1] We recall that the "nPN approximation" means the obtention of the terms of order $(v/c)^{2n} \sim (Gm/c^2r)^n$ in the equations of motion.

II. REDUCTION OF THE 3PN HIGHER-ORDER HAMILTONIAN

It was shown some years ago [7] that, in most coordinate systems, the conservative part of the PN-expanded equations of motion of two body systems, say $\ddot{\mathbf{x}}_a = \boldsymbol{\mathcal{A}}_a(\mathbf{x}_b, \dot{\mathbf{x}}_b)$, where $a, b = 1, 2$ and where $\boldsymbol{\mathcal{A}} = \mathbf{A}_0 + c^{-2}\mathbf{A}_2 + c^{-4}\mathbf{A}_4 + c^{-6}\mathbf{A}_6 + \ldots$, do not follow from any *ordinary* Lagrangian $L(\mathbf{x}_a, \dot{\mathbf{x}}_a)$. For instance, in harmonic coordinates, and at the 2PN level, one needs to consider an acceleration-dependent Lagrangian $L_{2\mathrm{PN}}^{\mathrm{harmonic}}(\mathbf{x}_a, \dot{\mathbf{x}}_a, \ddot{\mathbf{x}}_a)$ [1]. However, it was shown in Ref. [8], and, more generally, in Ref. [7], that any higher-order PN-expanded Lagrangian $L(\mathbf{x}_a, \dot{\mathbf{x}}_a, \ddot{\mathbf{x}}_a, \ldots)$ (where higher derivatives enter only perturbatively) can be reduced to an ordinary Lagrangian $L'(\mathbf{x}'_a, \dot{\mathbf{x}}'_a)$ by a suitable (higher-order) *contact transformation* $\mathbf{x}'_a(t) = \mathbf{x}_a(t) - \boldsymbol{\epsilon}_a(\mathbf{x}_b, \dot{\mathbf{x}}_b, \ldots)$. At the 2PN level the class of coordinates where the dynamics admit an ordinary Lagrangian is rather restricted [7], but it includes in particular the ADM coordinates [9,10]. At the 3PN level, Jaranowski and Schäfer, who worked within the ADM canonical formalism, have found that the (conservative) ADM dynamics could not be derived from an ordinary Hamiltonian $H(\mathbf{x}_a, \mathbf{p}_a)$ (equivalent to an ordinary Lagrangian $L(\mathbf{x}_a, \dot{\mathbf{x}}_a)$), but that instead it could be derived from a certain higher-order Hamiltonian $\widetilde{H}(\mathbf{x}_a, \mathbf{p}_a, \dot{\mathbf{x}}_a, \dot{\mathbf{p}}_a)$. [This higher-order matter Hamiltonian is defined by eliminating the field variables h_{ij}^{TT}, $\dot{h}_{ij}^{\mathrm{TT}}$ in a certain Routh (i.e., mixed) functional $R(\mathbf{x}_a, \mathbf{p}_a, h_{ij}^{\mathrm{TT}}, \dot{h}_{ij}^{\mathrm{TT}})$; see Eq. (33) of Ref. [2].] The meaning of this higher-order matter Hamiltonian $\widetilde{H}(\mathbf{x}_a, \mathbf{p}_a, \dot{\mathbf{x}}_a, \dot{\mathbf{p}}_a)$ is that the equations of motion of the matter can be written (after elimination of the TT variables) as

$$\dot{\mathbf{x}}_a = \frac{\delta \widetilde{H}(\mathbf{x}_b, \mathbf{p}_b, \dot{\mathbf{x}}_b, \dot{\mathbf{p}}_b)}{\delta \mathbf{p}_a}, \quad \dot{\mathbf{p}}_a = -\frac{\delta \widetilde{H}(\mathbf{x}_b, \mathbf{p}_b, \dot{\mathbf{x}}_b, \dot{\mathbf{p}}_b)}{\delta \mathbf{x}_a}, \tag{2.1}$$

where $\delta/\delta\mathbf{p}_a$ and $\delta/\delta\mathbf{x}_a$ denote functional derivatives:

$$\frac{\delta \widetilde{H}}{\delta \mathbf{p}_a} \equiv \frac{\partial \widetilde{H}}{\partial \mathbf{p}_a} - \frac{d}{dt}\left(\frac{\partial \widetilde{H}}{\partial \dot{\mathbf{p}}_a}\right), \quad \frac{\delta \widetilde{H}}{\delta \mathbf{x}_a} \equiv \frac{\partial \widetilde{H}}{\partial \mathbf{x}_a} - \frac{d}{dt}\left(\frac{\partial \widetilde{H}}{\partial \dot{\mathbf{x}}_a}\right). \tag{2.2}$$

It is easily seen that the Hamilton-like equations of motion (2.1) are equivalent to the Euler-Lagrange equations derived by extremizing the action functional

$$\widetilde{S}[\mathbf{x}_a(t), \mathbf{p}_a(t)] = \int dt\, \widetilde{L}(\mathbf{x}_b, \mathbf{p}_b, \dot{\mathbf{x}}_b, \dot{\mathbf{p}}_b), \tag{2.3}$$

where

$$\widetilde{L}(\mathbf{x}_b, \mathbf{p}_b, \dot{\mathbf{x}}_b, \dot{\mathbf{p}}_b) \equiv \mathbf{p}_a \dot{\mathbf{x}}_a - \widetilde{H}(\mathbf{x}_b, \mathbf{p}_b, \dot{\mathbf{x}}_b, \dot{\mathbf{p}}_b). \tag{2.4}$$

Indeed, we have

$$\frac{\delta \widetilde{L}}{\delta \mathbf{p}_a} \equiv \dot{\mathbf{x}}_a - \frac{\delta \widetilde{H}}{\delta \mathbf{p}_a}, \quad \frac{\delta \widetilde{L}}{\delta \mathbf{x}_a} \equiv -\dot{\mathbf{p}}_a - \frac{\delta \widetilde{H}}{\delta \mathbf{x}_a}. \tag{2.5}$$

To derive the dynamical invariants of the 3PN equations of motion it is convenient to introduce new coordinates (in phase-space $(\mathbf{x}_a, \mathbf{p}_a)$),

$$\mathbf{x}'_a = \mathbf{x}_a + \delta\mathbf{x}_a, \quad \mathbf{p}'_a = \mathbf{p}_a + \delta\mathbf{p}_a, \tag{2.6}$$

such that the equations of motion for $(\mathbf{x}'_a, \mathbf{p}'_a)$ become some ordinary Hamilton equations

$$\dot{\mathbf{x}}'_a = \frac{\partial H'(\mathbf{x}'_b, \mathbf{p}'_b)}{\partial \mathbf{p}'_a}, \quad \dot{\mathbf{p}}'_a = -\frac{\partial H'(\mathbf{x}'_b, \mathbf{p}'_b)}{\partial \mathbf{x}'_a}. \tag{2.7}$$

This is equivalent to requiring that the $(\mathbf{x}'_a, \mathbf{p}'_a)$ equations of motion derive from an action functional of the form

$$S'[\mathbf{x}'_a(t), \mathbf{p}'_a(t)] = \int dt\, L'(\mathbf{x}'_b, \mathbf{p}'_b, \dot{\mathbf{x}}'_b, \dot{\mathbf{p}}'_b), \tag{2.8}$$

where[2]

[2] As defined L' does not depend on $\dot{\mathbf{p}}'$, but, by symmetry, it is convenient to allow for such a dependence (which can be easily introduced by transforming $\mathbf{p}'\dot{\mathbf{x}}'$ by parts).

$$L'(\mathbf{x}'_b, \mathbf{p}'_b, \dot{\mathbf{x}}'_b, \dot{\mathbf{p}}'_b) \equiv \mathbf{p}'_a \dot{\mathbf{x}}'_a - H'(\mathbf{x}'_b, \mathbf{p}'_b). \tag{2.9}$$

When so expressed at the level of action functionals, the problem of reducing the 'higher-order' action $\widetilde{S}[\mathbf{x}_a(t), \mathbf{p}_a(t)]$ to an ordinary action $S'[\mathbf{x}'_a(t), \mathbf{p}'_a(t)]$ is quite similar to the problem of the order-reduction of (perturbative) higher-order actions $S[\mathbf{x}_a(t)] = \int dt\, L(\mathbf{x}_a, \dot{\mathbf{x}}_a, \ddot{\mathbf{x}}_a, \ldots)$ which was solved in full generality in Ref. [7]. It is then an easy task to adapt the techniques used in [7] to solve our present problem.

First, we note that, taking into account the fact that the Hamiltonian has the perturbative structure, $\widetilde{H}(\mathbf{x}_a, \mathbf{p}_a, \dot{\mathbf{x}}_a, \dot{\mathbf{p}}_a) = H_0(\mathbf{x}_a, \mathbf{p}_a) + c^{-2} H_2(\mathbf{x}_a, \mathbf{p}_a) + c^{-4} H_4(\mathbf{x}_a, \mathbf{p}_a) + c^{-6} H_6(\mathbf{x}_a, \mathbf{p}_a, \dot{\mathbf{x}}_a, \dot{\mathbf{p}}_a)$, the identities (2.5) for the variational derivatives of $\widetilde{L}(\mathbf{x}_a, \mathbf{p}_a, \dot{\mathbf{x}}_a, \dot{\mathbf{p}}_a)$ imply

$$\dot{\mathbf{x}}_a \equiv \mathbf{v}_{2\mathrm{PN}a}(\mathbf{x}, \mathbf{p}) + \frac{\delta \widetilde{L}}{\delta \mathbf{p}_a} + \mathcal{O}(c^{-6}) = \mathbf{v}_{\mathrm{N}a}(\mathbf{x}, \mathbf{p}) + \frac{\delta \widetilde{L}}{\delta \mathbf{p}_a} + \mathcal{O}(c^{-2}), \tag{2.10a}$$

$$\dot{\mathbf{p}}_a \equiv \mathbf{q}_{2\mathrm{PN}a}(\mathbf{x}, \mathbf{p}) - \frac{\delta \widetilde{L}}{\delta \mathbf{x}_a} + \mathcal{O}(c^{-6}) = \mathbf{q}_{\mathrm{N}a}(\mathbf{x}, \mathbf{p}) - \frac{\delta \widetilde{L}}{\delta \mathbf{x}_a} + \mathcal{O}(c^{-2}). \tag{2.10b}$$

Here $\mathbf{v}_{ia}$ and $\mathbf{q}_{ia}$ (with i = 2PN or N) denote some explicit functions of $\mathbf{x}$ and $\mathbf{p}$ which are the right-hand-sides of the usual Hamilton equations at the 2PN (or Newtonian) level. For instance, at the Newtonian level $\mathbf{v}_{\mathrm{N}a}(\mathbf{x}, \mathbf{p}) = \mathbf{p}_a / m_a$, $\mathbf{q}_{\mathrm{N}a}(\mathbf{x}, \mathbf{p}) = -G m_a m_b (\mathbf{x}_a - \mathbf{x}_b)/|\mathbf{x}_a - \mathbf{x}_b|^3$. Note that in Eqs. (2.10), and in the reasoning below, we are working 'off shell', i.e., we consider virtual motions which do not necessarily satisfy the equations of motion. [As we are using identities for action functionals, it is essential to work off shell.] Inserting the perturbative identities (2.10) in $\widetilde{H}(\mathbf{x}, \mathbf{p}, \dot{\mathbf{x}}, \dot{\mathbf{p}})$ and Taylor expanding yields the identity[3]

$$\widetilde{H}(\mathbf{x}, \mathbf{p}, \dot{\mathbf{x}}, \dot{\mathbf{p}}) \equiv \hat{H}(\mathbf{x}, \mathbf{p}) + \frac{\partial \widetilde{H}}{\partial \dot{\mathbf{x}}} \frac{\delta \widetilde{L}}{\delta \mathbf{p}} - \frac{\partial \widetilde{H}}{\partial \dot{\mathbf{p}}} \frac{\delta \widetilde{L}}{\delta \mathbf{x}} + \text{double-zeros} + \mathcal{O}(c^{-8}), \tag{2.11}$$

where $\hat{H}(\mathbf{x}, \mathbf{p})$ denotes the naive 'order-reduced' Hamiltonian obtained by using the (lower-order) equations of motion to eliminate the higher-order derivative terms (a wrong procedure in general):

$$\hat{H}(\mathbf{x}, \mathbf{p}) \equiv \widetilde{H}(\mathbf{x}, \mathbf{p}, \mathbf{v}_{\mathrm{N}}(\mathbf{x}, \mathbf{p}), \mathbf{q}_{\mathrm{N}}(\mathbf{x}, \mathbf{p})) + \mathcal{O}(c^{-8}). \tag{2.12}$$

[As indicated in Eq. (2.12), it is sufficient to use the Newtonian equations of motion because $\dot{\mathbf{x}}$ and $\dot{\mathbf{p}}$ enter only at the c^{-6} level.] The 'double-zeros' in Eq. (2.11) denote all the terms generated by the Taylor expansion which would be at least quadratic in $\delta \widetilde{L}/\delta \mathbf{x}$ and $\delta \widetilde{L}/\delta \mathbf{p}$. As is well known [11,7] such terms can be perturbatively neglected (even off shell) because they do not contribute to the equations of motion at the 3PN level.

If one inserts the identity (2.11) in the original action functional (2.3), one sees that $\widetilde{S}[\mathbf{x}, \mathbf{p}]$ has the desired ordinary form (2.8) modulo some extra terms which are *linear* in $\delta \widetilde{L}/\delta \mathbf{x}$ and $\delta \widetilde{L}/\delta \mathbf{p}$. As in Ref. [7] such terms can be eliminated by noticing that (to first order) the effect of the shift of dynamical variables (2.6) on the Lagrangian $\widetilde{L}(\mathbf{x}, \mathbf{p}, \dot{\mathbf{x}}, \dot{\mathbf{p}})$ reads (by virtue of the definition of functional derivatives)

$$\widetilde{L}(\mathbf{x}, \mathbf{p}, \dot{\mathbf{x}}, \dot{\mathbf{p}}) \equiv \widetilde{L}(\mathbf{x}', \mathbf{p}', \dot{\mathbf{x}}', \dot{\mathbf{p}}') - \frac{\delta \widetilde{L}}{\delta \mathbf{x}} \delta \mathbf{x} - \frac{\delta \widetilde{L}}{\delta \mathbf{p}} \delta \mathbf{p} + \frac{d}{dt} Q(\delta \mathbf{x}, \delta \mathbf{p}), \tag{2.13}$$

where $Q(\delta \mathbf{x}, \delta \mathbf{p})$ is some linear form in $\delta \mathbf{x}$ and $\delta \mathbf{p}$. [It is sufficient to work to linear order because $\delta \mathbf{x}$ and $\delta \mathbf{p}$ are $\mathcal{O}(c^{-6})$.]

By combining the two identities (2.11) and (2.13) we find that, if we define the ordinary Lagrangian (considered in phase-space) $\hat{L}$, associated to the ordinary (naively reduced) Hamiltonian $\hat{H}(\mathbf{x}, \mathbf{p})$, Eq. (2.12),

$$\hat{L}(\mathbf{x}, \mathbf{p}, \dot{\mathbf{x}}, \dot{\mathbf{p}}) \equiv \mathbf{p}_a \dot{\mathbf{x}}_a - \hat{H}(\mathbf{x}, \mathbf{p}), \tag{2.14}$$

we have the identity

[3] In Eq. (2.11) and elsewhere, we abbreviate the notation by suppressing the (summed over) indices in $\dot{\mathbf{x}} = \dot{x}^i_a$, $\mathbf{p} = p_{ai}$, etc.

$$\widetilde{L}(\mathbf{x},\mathbf{p},\dot{\mathbf{x}},\dot{\mathbf{p}}) \equiv \hat{L}(\mathbf{x}',\mathbf{p}',\dot{\mathbf{x}}',\dot{\mathbf{p}}') - \frac{\delta\widetilde{L}}{\delta\mathbf{x}}\left(\delta\mathbf{x} - \frac{\partial\widetilde{H}}{\partial\dot{\mathbf{p}}}\right) - \frac{\delta\widetilde{L}}{\delta\mathbf{p}}\left(\delta\mathbf{p} + \frac{\partial\widetilde{H}}{\partial\dot{\mathbf{x}}}\right) + \frac{d}{dt}Q(\delta\mathbf{x},\delta\mathbf{p}) + \text{double-zeros} + \mathcal{O}(c^{-8}). \tag{2.15}$$

Therefore, if we shift the phase-space coordinates by defining

$$\mathbf{x}'_a - \mathbf{x}_a \equiv \delta\mathbf{x}_a = \frac{\partial\widetilde{H}}{\partial\dot{\mathbf{p}}_a}, \quad \mathbf{p}'_a - \mathbf{p}_a \equiv \delta\mathbf{p}_a = -\frac{\partial\widetilde{H}}{\partial\dot{\mathbf{x}}_a}, \tag{2.16}$$

we find (noticing that both total differentials, and double-zeros, are negligible in action functionals) that the original equations of motion (2.1) are transformed, when rewritten in $(\mathbf{x}',\mathbf{p}')$ coordinates, into the Euler-Lagrange equations of the 'ordinary' phase-space Lagrangian $\hat{L}(\mathbf{x}',\mathbf{p}',\dot{\mathbf{x}}',\dot{\mathbf{p}}')$, i.e. into ordinary Hamilton equations

$$\dot{\mathbf{x}}' = \frac{\partial\hat{H}(\mathbf{x}',\mathbf{p}')}{\partial\mathbf{p}'} + \mathcal{O}(c^{-8}), \quad \dot{\mathbf{p}}' = -\frac{\partial\hat{H}(\mathbf{x}',\mathbf{p}')}{\partial\mathbf{x}'} + \mathcal{O}(c^{-8}). \tag{2.17}$$

Summarizing: it is licit to naively reduce the higher-order original Hamiltonian $\widetilde{H}(\mathbf{x},\mathbf{p},\dot{\mathbf{x}},\dot{\mathbf{p}})$ by replacing the lower-order equations of motion in the offending derivatives $\dot{\mathbf{x}}$, $\dot{\mathbf{p}}$ (thereby defining the reduced Hamiltonian $\hat{H}(\mathbf{x},\mathbf{p})$, Eq. (2.12)), if one adds the correcting information that the ordinary Hamilton equations defined by the reduced $\hat{H}(\mathbf{x},\mathbf{p})$ hold in the new phase-space coordinates $(\mathbf{x}',\mathbf{p}')$ defined by Eq. (2.16).

Let us note for completness that the conserved energy $\mathcal{E}' = \hat{H}(\mathbf{x}',\mathbf{p}')$ defined by the autonomous Hamiltonian $\hat{H}$ becomes, when expressed in the original variables

$$\mathcal{E}' = \hat{H}(\mathbf{x}',\mathbf{p}') = \hat{H}(\mathbf{x},\mathbf{p}) + \frac{\partial\hat{H}}{\partial\mathbf{x}}\frac{\partial\widetilde{H}}{\partial\dot{\mathbf{p}}} - \frac{\partial\hat{H}}{\partial\mathbf{p}}\frac{\partial\widetilde{H}}{\partial\dot{\mathbf{x}}} = \mathcal{E} + \mathcal{O}(c^{-8}), \tag{2.18}$$

where

$$\mathcal{E} = \widetilde{H}(\mathbf{x},\mathbf{p},\dot{\mathbf{x}},\dot{\mathbf{p}}) - \dot{\mathbf{x}}\frac{\partial\widetilde{H}}{\partial\dot{\mathbf{x}}} - \dot{\mathbf{p}}\frac{\partial\widetilde{H}}{\partial\dot{\mathbf{p}}} \tag{2.19}$$

is, indeed, easily checked to be a conserved quantity associated with the higher-order dynamics (2.1).

Let us now consider the explicit application of the previous results to the case at hand. Following [2] it is sufficient to consider the dynamics of the relative motion of a two-body system, considered in the center-of-mass frame ($\mathbf{p}_1 + \mathbf{p}_2 = 0$). It is convenient to work with the following reduced variables[4]

$$\mathbf{r} \equiv \frac{\mathbf{x}_1 - \mathbf{x}_2}{GM}, \quad \mathbf{p} \equiv \frac{\mathbf{p}_1}{\mu} = -\frac{\mathbf{p}_2}{\mu}, \quad \hat{t} \equiv \frac{t}{GM}, \quad \widehat{H}^{\rm NR} \equiv \frac{\widetilde{H}^{\rm NR}}{\mu}, \tag{2.20}$$

where

$$M \equiv m_1 + m_2, \quad \mu \equiv \frac{m_1 m_2}{M}, \quad \nu \equiv \frac{\mu}{M} = \frac{m_1 m_2}{(m_1+m_2)^2}. \tag{2.21}$$

In Eq. (2.20) the superscript NR denotes a 'non-relativistic' (higher-order) Hamiltonian, i.e. the Hamiltonian without the rest-mass contribution Mc^2. $\widehat{H}^{\rm NR}$ is, to start with, a function of $\mathbf{r}$, $\mathbf{p}$, $\dot{\mathbf{r}}$, and $\dot{\mathbf{p}}$. Here the dot denotes the reduced-time derivative:

$$\dot{\mathbf{r}} = \frac{d\mathbf{r}}{d\hat{t}} = \frac{d(\mathbf{x}_1 - \mathbf{x}_2)}{dt}, \quad \dot{\mathbf{p}} = \frac{d\mathbf{p}}{d\hat{t}} = \frac{G}{\nu}\frac{d\mathbf{p}_1}{dt} = -\frac{G}{\nu}\frac{d\mathbf{p}_2}{dt}. \tag{2.22}$$

From Eq. (2.16) above and Eq. (68) of [2] one finds that the coordinate shift needed to transform $\widehat{H}^{\rm NR}(\mathbf{r},\mathbf{p},\dot{\mathbf{r}},\dot{\mathbf{p}})$ into an ordinary Hamiltonian reads (on shell[5], i.e. by using the (Newtonian) equations of motion after the differentiations exhibited in Eq. (2.16))

[4] Note that [2] use units where $16\pi G = 1$.

[5] Working on shell here is equivalent to neglecting some double-zero terms, see, e.g. Ref. [7].

$$\delta \mathbf{r} \equiv \mathbf{r}' - \mathbf{r} = \frac{\partial \widehat{H}^{\rm NR}}{\partial \dot{\mathbf{p}}}\bigg|_{\rm on\ shell} = \frac{1}{c^6}\left\{\left[\frac{1}{8}\nu^2\left((\mathbf{n}\cdot\mathbf{p})^4 - (\mathbf{p}^2)^2\right) + \frac{1}{24}\left((19-26\nu)\nu\,(\mathbf{n}\cdot\mathbf{p})^2 - 5(13+4\nu)\nu\,\mathbf{p}^2\right)\frac{1}{r}\right]\mathbf{n}\right.$$

$$\left. + \frac{1}{12}\left[\nu^2\left(3\mathbf{p}^2 + (\mathbf{n}\cdot\mathbf{p})^2\right)(\mathbf{n}\cdot\mathbf{p}) - (14-\nu)\nu\,(\mathbf{n}\cdot\mathbf{p})\frac{1}{r}\right]\mathbf{p}\right\}, \tag{2.23a}$$

$$\delta \mathbf{p} \equiv \mathbf{p}' - \mathbf{p} = -\frac{\partial \widehat{H}^{\rm NR}}{\partial \dot{\mathbf{r}}}\bigg|_{\rm on\ shell} = \frac{1}{c^6}\left\{\left[\frac{1}{8}\nu^3\left((\mathbf{p}^2)^2 + 2(\mathbf{n}\cdot\mathbf{p})^2\mathbf{p}^2 + 5(\mathbf{n}\cdot\mathbf{p})^4\right)(\mathbf{n}\cdot\mathbf{p})\frac{1}{r}\right.\right.$$

$$\left. - \frac{1}{48}\left(3(1-9\nu)\nu\,\mathbf{p}^2 + 5(17-29\nu)\nu\,(\mathbf{n}\cdot\mathbf{p})^2\right)(\mathbf{n}\cdot\mathbf{p})\frac{1}{r^2} + \frac{1}{512}\left(11408 - 915\pi^2 + 36(48-5\pi^2)\nu\right)\nu\,(\mathbf{n}\cdot\mathbf{p})\frac{1}{r^3}\right]\mathbf{n}$$

$$+ \left[-\frac{1}{8}\nu^3\left((\mathbf{p}^2)^2 + 2(\mathbf{n}\cdot\mathbf{p})^2\mathbf{p}^2 + 5(\mathbf{n}\cdot\mathbf{p})^4\right)\frac{1}{r} + \frac{1}{16}\left((4-15\nu)\nu\,\mathbf{p}^2 + (6+7\nu)\nu\,(\mathbf{n}\cdot\mathbf{p})^2\right)\frac{1}{r^2}\right.$$

$$\left.\left. + \frac{1}{1536}\left(15(61\pi^2 - 880) + 4(45\pi^2 - 592)\nu\right)\nu\frac{1}{r^3}\right]\mathbf{p}\right\}. \tag{2.23b}$$

Note again that $\delta\mathbf{r}$ and $\delta\mathbf{p}$ are of 3PN order.

III. ORDER-REDUCED 3PN HAMILTONIAN

As explained above the phase-space coordinate transformation (2.23) maps the original higher-order 3PN ADM dynamics onto ordinary Hamilton equations, with an Hamiltonian $\overline{H}(\mathbf{r}', \mathbf{p}')$ defined by the 'naive' procedure (2.12), i.e. by using in $\widehat{H}^{\rm NR}(\mathbf{r}, \mathbf{p}, \dot{\mathbf{r}}, \dot{\mathbf{p}})$ the following replacement rules (in our reduced units where $\widehat{H}^{\rm NR}_{\rm Newtonian}(\mathbf{r}, \mathbf{p}) = \mathbf{p}^2/2 - 1/r$, with $r \equiv |\mathbf{r}|$)

$$\mathbf{r} \to \mathbf{r}', \quad \mathbf{p} \to \mathbf{p}', \quad \dot{\mathbf{r}} \to \mathbf{p}', \quad \dot{\mathbf{p}} \to -\frac{\mathbf{r}'}{r'^3}. \tag{3.1}$$

To simplify the writing we shall henceforth drop all the primes (but the reader should remember that we henceforth work in the shifted coordinate system $(\mathbf{r}', \mathbf{p}')$). We also drop the overbar, on the Hamiltonian, indicating that we have used the replacement rules (3.1). Finally, using Eqs. (68) and (71) of [2], we obtain the following ordinary Hamiltonian (with $\mathbf{n} \equiv \mathbf{r}/r$)

$$\widehat{H}^{\rm NR}(\mathbf{r}, \mathbf{p}) = \widehat{H}_{\rm N}(\mathbf{r}, \mathbf{p}) + \frac{1}{c^2}\widehat{H}_{\rm 1PN}(\mathbf{r}, \mathbf{p}) + \frac{1}{c^4}\widehat{H}_{\rm 2PN}(\mathbf{r}, \mathbf{p}) + \frac{1}{c^6}\widehat{H}_{\rm 3PN}(\mathbf{r}, \mathbf{p}), \tag{3.2}$$

where

$$\widehat{H}_{\rm N}(\mathbf{r}, \mathbf{p}) = \frac{\mathbf{p}^2}{2} - \frac{1}{r}, \tag{3.3}$$

$$\widehat{H}_{\rm 1PN}(\mathbf{r}, \mathbf{p}) = \frac{1}{8}(3\nu - 1)(\mathbf{p}^2)^2 - \frac{1}{2}\left[(3+\nu)\mathbf{p}^2 + \nu(\mathbf{n}\cdot\mathbf{p})^2\right]\frac{1}{r} + \frac{1}{2r^2}, \tag{3.4}$$

$$\widehat{H}_{\rm 2PN}(\mathbf{r}, \mathbf{p}) = \frac{1}{16}\left(1 - 5\nu + 5\nu^2\right)(\mathbf{p}^2)^3 + \frac{1}{8}\left[\left(5 - 20\nu - 3\nu^2\right)(\mathbf{p}^2)^2 - 2\nu^2(\mathbf{n}\cdot\mathbf{p})^2\mathbf{p}^2 - 3\nu^2(\mathbf{n}\cdot\mathbf{p})^4\right]\frac{1}{r}$$

$$+ \frac{1}{2}\left[(5+8\nu)\mathbf{p}^2 + 3\nu(\mathbf{n}\cdot\mathbf{p})^2\right]\frac{1}{r^2} - \frac{1}{4}(1+3\nu)\frac{1}{r^3}, \tag{3.5}$$

$$\widehat{H}_{\rm 3PN}(\mathbf{r}, \mathbf{p}) = \frac{1}{128}\left(-5 + 35\nu - 70\nu^2 + 35\nu^3\right)(\mathbf{p}^2)^4$$

$$+ \frac{1}{16}\left[\left(-7 + 42\nu - 53\nu^2 - 5\nu^3\right)(\mathbf{p}^2)^3 + (2-3\nu)\nu^2(\mathbf{n}\cdot\mathbf{p})^2(\mathbf{p}^2)^2 + 3(1-\nu)\nu^2(\mathbf{n}\cdot\mathbf{p})^4\mathbf{p}^2 - 5\nu^3(\mathbf{n}\cdot\mathbf{p})^6\right]\frac{1}{r}$$

$$+\left[\frac{1}{16}\left(-27+136\nu+109\nu^2\right)(\mathbf{p}^2)^2+\frac{1}{16}(17+30\nu)\nu(\mathbf{n}\cdot\mathbf{p})^2\mathbf{p}^2+\frac{1}{12}(5+43\nu)\nu(\mathbf{n}\cdot\mathbf{p})^4\right]\frac{1}{r^2}$$

$$+\left\{\left[-\frac{25}{8}+(\frac{1}{64}\pi^2-\frac{335}{48})\nu-\frac{55}{12}\nu^2\right]\mathbf{p}^2+\left(-\frac{85}{16}-\frac{3}{64}\pi^2+\frac{27}{8}\nu\right)\nu(\mathbf{n}\cdot\mathbf{p})^2\right\}\frac{1}{r^3}$$

$$+\left[\frac{1}{8}+(\frac{109}{12}-\frac{21}{32}\pi^2)\nu\right]\frac{1}{r^4}+\omega_{\rm kinetic}\left(\mathbf{p}^2-3(\mathbf{n}\cdot\mathbf{p})^2\right)\frac{\nu^2}{r^3}+\omega_{\rm static}\frac{\nu}{r^4}. \tag{3.6}$$

The parameters $\omega_{\rm kinetic}$ and $\omega_{\rm static}$ appearing in the 3PN Hamiltonian $\widehat{H}_{\rm 3PN}$ parametrize the existence of *ambiguities* in the regularization (as it is presently performed) of some of the divergent integrals making up the Hamiltonian.

It was shown by Damour [12] that the internal structure of the compact bodies making up a binary system (e.g. a neutron star versus a black hole) start influencing the dynamics only at the 5PN level (G^6/c^{10}; see Eq. (19) in Sec. 5 of Ref. [12]). Therefore, one expects that the present 3PN ambiguities are of technical nature, and not linked to real physical ambiguities. The best way to resolve these ambiguities would be to work out in detail, at the 3PN level, the general matching method outlined in Ref. [12], and applied there at the 2PN level. However, the technical difficultities of working at the 3PN level are such that this route has not yet been attempted.

The 'kinetic ambiguity' $\omega_{\rm kinetic}\nu^2\left(\mathbf{p}^2-3(\mathbf{n}\cdot\mathbf{p})^2\right)/r^3$ (proportional to the kinetic energy $\mathbf{p}^2$) was explicitly introduced in Ref. [2] (see Eq. (69) there; with $\omega^{\rm there}$ corresponding to $\omega^{\rm here}_{\rm kinetic}$ modulo the shift of normalization discussed below). The 'static ambiguity' $\omega_{\rm static}\nu/r^4$ was discussed in Ref. [13]. In the present paper, we normalize the static ambiguity such that the value $\omega_{\rm static}=0$ corresponds to the static interaction[6] between two 'Brill-Lindquist black holes' (considered instantaneously at rest; see [13]). The normalization of the kinetic ambiguity used in Eq. (3.6) of this paper also differs from that used in Eq. (71) of [2]. The motivation for this new normalization is given in Appendix A of the present paper, where we calculate, following the route of Ref. [2], a new 'reference' Hamiltonian which corresponds to this normalization. In terms of these two normalizations, the Hamiltonian explicitly written in [2] corresponds to the values $\omega_{\rm static}=1/8$ and $\omega_{\rm kinetic}=7/16+\omega$; this means that (after having applied the replacement rule (3.1) and dropped the primes)

$$\widehat{H}_{\rm 3PN}^{\rm this\ paper}(\mathbf{r},\mathbf{p})=\widehat{H}_{\rm 3PN}^{\rm Ref.\,[2]}(\mathbf{r},\mathbf{p})+\left(\omega_{\rm static}-\frac{1}{8}\right)\frac{\nu}{r^4}+\left(\omega_{\rm kinetic}-\frac{7}{16}-\omega\right)\left(\mathbf{p}^2-3(\mathbf{n}\cdot\mathbf{p})^2\right)\frac{\nu^2}{r^3}. \tag{3.7}$$

Though the two parameters $\omega_{\rm static}$ and $\omega_{\rm kinetic}$ appear separately in Eq. (3.6), all the dynamical invariants of the 3PN Hamiltonian involve only the combination

$$\sigma(\nu)\equiv\nu\omega_{\rm static}+\nu^2\omega_{\rm kinetic}. \tag{3.8}$$

Our results below will verify explicitly that only the combination σ appears, but it is, in fact, easy to understand why. Indeed, as we shall calculate the dynamical invariants of $H(\mathbf{r},\mathbf{p})$, our results would be the same if we transformed H by an arbitrary canonical transformation. If we consider 'a small' canonical transformation of order $1/c^6$, it is enough to work at linear order. At linear order a canonical transformation is parametrized by an arbitrary generating function $g(\mathbf{r},\mathbf{p})$, and its effect on the Hamiltonian is to change it by the Poisson bracket $\{g,H\}$:

$$\delta H(\mathbf{r},\mathbf{p})=\{g,H\}=\frac{\partial g}{\partial x^i}\frac{\partial H}{\partial p_i}-\frac{\partial g}{\partial p_i}\frac{\partial H}{\partial x^i}=p_i\frac{\partial g}{\partial x^i}-\frac{x^i}{r^3}\frac{\partial g}{\partial p_i}+\mathcal{O}(g/c^2). \tag{3.9}$$

If we choose $g(\mathbf{r},\mathbf{p})=\lambda\mathbf{r}\cdot\mathbf{p}/r^3$ we find

$$\delta H=\frac{\lambda}{r^3}\left(\mathbf{p}^2-3(\mathbf{n}\cdot\mathbf{p})^2\right)-\frac{\lambda}{r^4}. \tag{3.10}$$

Therefore by choosing (for instance) $\lambda=-\nu^2\omega_{\rm kinetic}$, we see that we can eliminate $\omega_{\rm kinetic}$ at the cost of replacing $\nu\omega_{\rm static}$ by $\nu\omega_{\rm static}-\lambda=\nu\omega_{\rm static}+\nu^2\omega_{\rm kinetic}$.

An important issue, when discussing the consequences of the 3PN Hamiltonian (3.2), is the influence of the lack of precise knowledge of the combination σ, Eq. (3.8), on physical observables. First, let us emphasize that, among

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[6] By 'static interaction' we mean the part of the Hamiltonian which remains when setting to zero both the momenta $\mathbf{p}_1$, $\mathbf{p}_2$ *and* the independent gravitational-wave degrees of freedom $h^{\rm TT}_{ij}$, $\pi^{ij\,\rm TT}$ (time-symmetric conformally flat data).

the hundreds of contributions to the 3PN Hamiltonian which have been computed in Ref. [2], most of them, though they are in general given by a divergent integral, seem to be regularizable in an unambigous manner. Indeed, if one considers *separately* the divergences near one particle (say in a volume V_1 near particle 1), and regularizes them 'à la Riesz', i.e. by introducing a regularizing factor $(|\mathbf{x}-\mathbf{x}_1|/l_1)^{\epsilon_1} = (r_1/l_1)^{\epsilon_1}$ in the integrand, the analytic continuation in ϵ_1 of the regularized integral $I_1(\epsilon_1) = \int_{V_1} d^3x\,(r_1/l_1)^{\epsilon_1} F(\mathbf{x},\mathbf{x}_1,\mathbf{x}_2)$ does not contain a pole $\propto 1/\epsilon_1$ for most terms. This suggests that the well-defined analytic continuation of $I_1(\epsilon_1)$ down to $\epsilon_1 = 0$ defines, without apparent ambiguity, the regularized value of $\int_{V_1} d^3x\, F(\mathbf{x},\mathbf{x}_1,\mathbf{x}_2)$. [In the notation of Appendix B of [2] we are considering that $\nu^{JS} = 0$ (i.e. $\epsilon_2 = \nu^{JS}\epsilon = 0$), in a V_1-restricted integral which behaves as $A_1 + C_1\nu^{JS}/\mu^{JS} = A_1 + C_1\epsilon_2/\epsilon_1$, before taking the limit $\epsilon_1 = \mu^{JS}\epsilon \to 0$.]

However, a limited class of 'dangereous' integrals involve a simple pole as $\epsilon_1 \to 0$: $I_1(\epsilon_1) = Z_1\big(\epsilon_1^{-1} + \ln(R_1/l_1)\big) + A_1$ (where the 'infrared' lengthscale R_1 is linked to the size of the volume V_1). A remarkable fact (emphasized in Section IV of [2]) is, however, that the complete combination of dangerous integrals appearing in $\widetilde{H}_{3PN}$ is such that all the pole terms cancel: $\sum Z_1 = 0$. This also implies that the logarithms depending on the 'ultraviolet' regularizing length l_1 cancel in the Hamiltonian [2]. In other words, the combination of dangerous integrals appearing in $\widetilde{H}_{3PN}$ is either 'finite' (convergent) or globally of a 'non dangerous' type. This is good news, but this still leaves an ambiguity in the finite value of $\sum I_1(\epsilon_1)$ because it was noticed in [2] that the final regularized result depends on the way one writes the 'bare' integrand $F(\mathbf{x},\mathbf{x}_1,\mathbf{x}_2)$ (when transforming it using standard rules: integration by parts, and Leibniz's rule). In addition to this ambiguity linked to a subset of divergent integrals, there are also ambiguities in the 'contact' terms in the Hamiltonian (of the type $\int d^3x\, \delta(\mathbf{x}-\mathbf{x}_1) S(\mathbf{x},\mathbf{x}_1,\mathbf{x}_2)$). One needs to regularize the (in general singular) limit $\lim_{\mathbf{x}\to\mathbf{x}_1} S(\mathbf{x},\mathbf{x}_1,\mathbf{x}_2)$. In [2] one used an Hadamard-like 'partie-finie' prescription (Pf$_1$) for doing that. This prescription is, however, ambiguous at 3PN, notably because $\mathrm{Pf}_1(\phi_{(2)}^4) \neq [\mathrm{Pf}_1(\phi_{(2)})]^4$ [13], where $\phi_{(2)}$ denotes the Newtonian potential. As said above, the final ambiguities in the Hamiltonian concern only two quite specific types of terms, parametrized by $\omega_{\rm static}$ and $\omega_{\rm kinetic}$ in Eq. (3.6).

In Appendix A of this paper, we discuss in more detail these ambiguities, and, we try to estimate what are the corresponding plausible ranges of values of the two ambiguity parameters $\omega_{\rm static}$ and $\omega_{\rm kinetic}$. For instance, when transforming (e.g. by integration by parts) the divergent integrands we generate some (rational) values for $\omega_{\rm static}$ and $\omega_{\rm kinetic}$. By doing this in various ways, we get an idea of the range of values that these parameters are likely to be in. The final result of Appendix A below is

$$-10 \lesssim \omega_{\rm static} \lesssim 10, \quad -10 \lesssim \omega_{\rm kinetic} \lesssim 10. \tag{3.11}$$

As the symmetric mass ratio $\nu \equiv m_1 m_2/(m_1+m_2)^2$ ranges between 0 and 1/4, the ranges (3.11) imply that $-3.125 \lesssim \sigma(\nu) \lesssim 3.125$. In the following, we shall therefore consider as *fiducial* range of variation for the (not yet known) combination σ the simple range

$$-3 \leq -12\nu \leq \sigma(\nu) \leq 12\nu \leq 3. \tag{3.12}$$

IV. DYNAMICAL INVARIANTS OF THE 3PN HAMILTONIAN

In this section we derive a complete (and, in fact, overcomplete) set of *invariant* functions of the 3PN dynamics. Only such functions enter the principal *observables* that can be measured from infinity (say, by gravitational wave observations). However, not all the invariants we derive here can be considered as being directly observable. In a subsequent paper, we shall discuss in detail one of the most important observable: the Last Stable (circular) Orbit.

We follow closely a work of Damour and Schäfer [14] in which they derived the invariants of the 2PN dynamics. One first uses the invariance of the Hamiltonian under time translations and spatial rotations. This yields the conserved quantities

$$E \equiv \frac{\mathcal{E}^{\rm NR}}{\mu} \equiv \widehat{H}^{\rm NR}(\mathbf{r},\mathbf{p}), \quad \mathbf{j} \equiv \frac{\mathbf{J}}{\mu G M} = \mathbf{r}\times\mathbf{p}. \tag{4.1}$$

Here $\mathcal{E}^{\rm NR}$ denotes the total 'non relativistic' energy (without rest-mass contribution), and $\mathbf{J}$ the total angular momentum of the binary system in the center of mass frame. Using the Hamilton-Jacobi approach, the motion in the plane of the relative trajectory is obtained, in polar coordinates (r,ϕ), by separating the variables $\hat{t} \equiv t/(GM)$ and ϕ in the reduced planar action

$$\widehat{S} \equiv \frac{S}{\mu G M} = -E\hat{t} + j\phi + \int dr\sqrt{R(r,E,j)}. \tag{4.2}$$

Here $j \equiv |\mathbf{j}|$ and $R(r, E, j)$ is an 'effective potential' for the radial motion which is obtained by solving the first equation (4.1) for $p_r^2 \equiv (\mathbf{n}\cdot\mathbf{p})^2$ after having replaced $\mathbf{p}^2$ by

$$\mathbf{p}^2 \equiv (\mathbf{n}\cdot\mathbf{p})^2 + (\mathbf{n}\times\mathbf{p})^2 = p_r^2 + \frac{j^2}{r^2}. \tag{4.3}$$

Working iteratively in the small parameter c^{-2}, and consistently neglecting all terms $\mathcal{O}(c^{-8})$, one finds that $R(r, E, j)$ is given, at 3PN order, by the following seventh-degree polynomial in $1/r$:

$$R(r, E, j) = A + \frac{2B}{r} + \frac{C}{r^2} + \frac{D_1^{1\mathrm{PN}}}{r^3} + \frac{D_2^{2\mathrm{PN}}}{r^4} + \frac{D_3^{2\mathrm{PN}}}{r^5} + \frac{D_4^{3\mathrm{PN}}}{r^6} + \frac{D_5^{3\mathrm{PN}}}{r^7}. \tag{4.4}$$

The coefficients A, B, C start at Newtonian order, while the extra terms D_i/r^{i+2} start at the PN order indicated as superscript. All the coefficients A, B, C, D_i are polynomials in E and j^2. Their explicit expressions are given in Appendix B.

The Hamilton-Jacobi theory shows that the observables of the 3PN motion are deducible from the (reduced) 'radial action integral'

$$i_r(E, j) \equiv \frac{2}{2\pi}\int_{r_{\min}}^{r_{\max}} dr\sqrt{R(r, E, j)}. \tag{4.5}$$

For instance, the periastron-to-periastron period P and the periastron advance $\Delta\Phi \equiv \Phi - 2\pi$ per orbit are obtained by differentiating the radial action integral:

$$\frac{P}{2\pi GM} = \frac{\partial}{\partial E} i_r(E, j), \tag{4.6}$$

$$\frac{\Phi}{2\pi} = 1 + \frac{\Delta\Phi}{2\pi} = -\frac{\partial}{\partial j} i_r(E, j). \tag{4.7}$$

To evaluate the invariant function $i_r(E, j)$ we follow Ref. [14], which was itself following a method devised by Sommerfeld [15] within the context of the 'old theory of quanta'. This method is explained in detail in the Appendix B of Ref. [14]. The basic idea is the following: define $Q(r) \equiv A + 2B/r + C/r^2$ and consider the integral

$$I(\epsilon) \equiv \frac{2}{2\pi}\int_{r_1(\epsilon)}^{r_2(\epsilon)} dr\sqrt{Q(r) + \epsilon\sum_n \frac{D_n}{r^{n+2}}}. \tag{4.8}$$

Here ϵ is a formal expansion parameter (actually in the final calculations, one takes into account the fact that the higher D_n's are multiplied by ϵ^2 or ϵ^3, with $\epsilon \sim 1/c^2$ being in factor of $D_1^{1\mathrm{PN}}$) and one wishes to compute the expansion of $I(\epsilon)$ as $\epsilon \to 0$: $I(\epsilon) = I_0 + \epsilon I_1 + \epsilon^2 I_2 + \epsilon^3 I_3 + \mathcal{O}(\epsilon^4)$. To start with, the limits of integration, $r_1(\epsilon)$ and $r_2(\epsilon)$, are the two exact (ϵ-dependent) real roots of $R(r) = Q(r) + \epsilon\sum D_n/r^{n+2}$. [We work in the case where $A < 0$, $B > 0$, and $C < 0$.] The idea is to consider the function $\sqrt{R(r)}$ as a complex analytic function defined in a suitably cut complex r-plane: with, say, a cut along the real segment linking $r_1(\epsilon)$ to $r_2(\epsilon)$, and additional cuts from, say, $-\infty$ to the other roots. This allows one to rewrite the real integral (4.8) as a contour integral

$$I(\epsilon) = \frac{1}{2\pi}\oint_C dr\sqrt{R(r, \epsilon)}, \tag{4.9}$$

where one should note the different numerical prefactor, and where C denotes any (counterclockwise, simply winding) contour enclosing the two real roots $r_1(\epsilon)$, $r_2(\epsilon)$, and avoiding all the cuts. [The phases of $r - r_1$ and $r - r_2$ are defined to be zero when r lies on the real axis on the right of r_2, while the phase of $\sqrt{A}$ is defined as $+\pi/2$.] If we keep the contour C away from the segment $[r_1(\epsilon), r_2(\epsilon)]$, we can now directly expand the integrand $\sqrt{R(r,\epsilon)}$ in the contour integral (4.9) in powers of ϵ. This generates the successive terms of the expansion $I(\epsilon) = I_0 + \epsilon I_1 + \epsilon^2 I_2 + \ldots$, with each term I_n being given by a contour integral made of a sum of contributions of the form

$$J_{q,m} = \frac{1}{2\pi}\oint_C dr\left(A + \frac{2B}{r} + \frac{C}{r^2}\right)^{\frac{1}{2}-q}\frac{1}{r^m}. \tag{4.10}$$

Each basic integral $J_{q,m}$ appears in the expansion of I multiplied by a coefficient which is a polynomial in the D_n's. [At any given PN order, there are only a finite number of integrals $J_{q,m}$ to compute; see below.]

There are then two ways to compute the $J_{q,m}$'s. The simplest (the one advocated by Sommerfeld) is to expand out the contour C (away from the natural cut $[r_1(0), r_2(0)]$ associated to the 'unperturbed' quadratic form $Ar^2+2Br+C$) until it is deformed into: (i) a *clockwise* contour C_0 around the origin $r=0$, and (ii) *anticlockwise* contour C_∞ at infinity. [Here, one considers that the J-integrals are defined in a newly cut plane, with a cut only along the segment $[r_1(0), r_2(0)]$.] The value of $J_{q,m}$ is then simply given by applying (twice) Cauchy's residue theorem: it is enough to read off the coefficients of $1/r$ in the two Laurent expansions of the integrand of Eq. (4.10) for $r \to 0$ and $r \to \infty$ (keeping track of phases and signs). The other way to compute the J's consists in shrinking down the contour C onto the real axis, so as to get (twice) a real integral from $r_1(0)+\eta$ to $r_2(0)-\eta$ (with $\eta > 0$), plus two circular integrals around $r_1(0)$ and $r_2(0)$. As shown in Appendix B of [14] one can then prove that the ϵ-expansion (Exp_ϵ) of $I(\epsilon)$ is simply given by

$$\mathrm{Exp}_\epsilon(I(\epsilon)) = \mathrm{Pf}\left[\frac{2}{2\pi}\int_{r_1(0)}^{r_2(0)} dr\, \mathrm{Exp}_\epsilon\left(\sqrt{R(r,\epsilon)}\right)\right], \tag{4.11}$$

where Pf denotes Hadamard's partie finie of the real r-integral. Each integral appearing in the formal ϵ-expansion of $\sqrt{R(r,\epsilon)}$ on the right-hand side of (4.11) is again the same combination of J-integrals as above, but now the J-integrals are real integrals along the segment $[r_1(0), r_2(0)]$, of which one must extract their 'partie finie'. The parties finies of all those real integrals are easily computed, e.g., by using any simple trigonometric parametrization of the radial variable ($r = a(1-e^2)/(1+e\cos v)$ or $r = a(1-e\cos u)$) to compute the indefinite integrals $\int dr[Q(r)]^{\frac{1}{2}-q} r^{-m}$.

The only integrals that one needs to compute at 3PN order are $J_{q,m}$ with $0 \le q \le 3$: when $q=0$, $m=0$; when $q=1$, $3 \le m \le 7$; when $q=2$, $6 \le m \le 8$; and when $q=3$, $m=9$. We have computed these integrals by the two methods indicated above, and checked that the results agree. The results are given in Appendix B below.

Finally, one must reexpand all the coefficients A, B, C, D_n (which contain various orders in $1/c^2$) to get the complete 3PN expansion of the radial action $i_r(E,j)$. The final result reads

$$\begin{aligned} i_r(E,j) = -j\Bigg\{ & 1 - \frac{1}{c^2}\frac{3}{j^2} - \frac{1}{c^4}\left[\frac{1}{4}(35-10\nu)\frac{1}{j^4} + \frac{1}{2}(15-6\nu)\frac{E}{j^2}\right] \\ & -\frac{1}{c^6}\left[\frac{3}{2}\big(i_1(\nu)-\sigma(\nu)\big)\frac{1}{j^6} + \big(i_2(\nu)-\sigma(\nu)\big)\frac{E}{j^4} + 3i_3(\nu)\frac{E^2}{j^2}\right]\Bigg\} \\ & + \frac{1}{\sqrt{-2E}}\left\{1 + \frac{1}{c^2}\frac{1}{4}(15-\nu)\,E + \frac{1}{c^4}\frac{1}{32}(35+30\nu+3\nu^2)\,E^2 - \frac{1}{c^6}i_4(\nu)\,E^3\right\}, \end{aligned} \tag{4.12}$$

where

$$i_1(\nu) = \frac{77}{2} + \left(\frac{41}{64}\pi^2 - \frac{125}{3}\right)\nu + \frac{83}{24}\nu^2, \tag{4.13a}$$

$$i_2(\nu) = \frac{105}{2} + \left(\frac{41}{64}\pi^2 - \frac{218}{3}\right)\nu + \frac{221}{24}\nu^2, \tag{4.13b}$$

$$i_3(\nu) = \frac{1}{4}(5 - 5\nu + 4\nu^2), \tag{4.13c}$$

$$i_4(\nu) = \frac{1}{128}(21 - 105\nu + 15\nu^2 + 5\nu^3). \tag{4.13d}$$

The differentiation (4.6) then leads to the following expression for the periastron-to-periastron period P

$$\begin{aligned} \frac{P}{2\pi GM} = \frac{1}{(-2E)^{3/2}}\Bigg\{ & 1 - \frac{1}{c^2}\frac{1}{4}(15-\nu)\,E \\ & + \frac{1}{c^4}\left[\frac{3}{2}(5-2\nu)\frac{(-2E)^{3/2}}{j} - \frac{3}{32}(35+30\nu+3\nu^2)\,E^2\right] \\ & + \frac{1}{c^6}\left[\big(i_2(\nu)-\sigma(\nu)\big)\frac{(-2E)^{3/2}}{j^3} - 3i_3(\nu)\frac{(-2E)^{5/2}}{j} + 5i_4(\nu)\,E^3\right]\Bigg\}, \end{aligned} \tag{4.14}$$

where $i_2(\nu)$, $i_3(\nu)$, and $i_4(\nu)$ are given in Eqs. (4.13b), (4.13c), and (4.13d), respectively. Similarly, the differentiation (4.7) yields, for the dimensionless parameter

$$k \equiv \frac{\Delta\Phi}{2\pi} = \frac{\Phi - 2\pi}{2\pi} \tag{4.15}$$

measuring the fractional periastron advance per orbit, the result

$$k = \frac{1}{c^2}\frac{3}{j^2}\left\{1 + \frac{1}{c^2}\left[\frac{5}{4}(7-2\nu)\frac{1}{j^2} + \frac{1}{2}(5-2\nu)\,E\right] + \frac{1}{c^4}\left[\frac{5}{2}\big(i_1(\nu)-\sigma(\nu)\big)\frac{1}{j^4} + \big(i_2(\nu)-\sigma(\nu)\big)\frac{E}{j^2} + 3i_3(\nu)\,E^2\right]\right\}, \tag{4.16}$$

where $i_1(\nu)$, $i_2(\nu)$, and $i_3(\nu)$ are given in Eqs. (4.13a), (4.13b), and (4.13c), respectively.

We shall also follow Ref. [14] in giving the Hamiltonian as a function of the Delaunay (reduced) action variables

$$n \equiv i_r + j = \frac{\mathcal{N}}{\mu GM}, \quad j = \frac{J}{\mu GM}, \quad m \equiv j_z = \frac{J_z}{\mu GM}. \tag{4.17}$$

In the quantum language, $\mathcal{N}/\hbar$ is the principal quantum number, $J/\hbar$ the total angular-momentum quantum number, and $J_z/\hbar$ the magnetic quantum number. [They are adiabatic invariants of the dynamics and they are (approximately) quantized in integers.] By rotational symmetry, the (reduced) magnetic quantum number m does not enter the Hamiltonian. By inverting Eq. (4.12) one finds

$$\begin{aligned}\widehat{H}(n,j,m) = -\frac{1}{2n^2}\Bigg\{&1 + \frac{1}{c^2}\left[\frac{6}{jn} - \frac{1}{4}(15-\nu)\frac{1}{n^2}\right]\\
&+\frac{1}{c^4}\left[\frac{5}{2}(7-2\nu)\frac{1}{j^3 n} + \frac{27}{j^2n^2} - \frac{3}{2}(35-4\nu)\frac{1}{jn^3} + \frac{1}{8}(145-15\nu+\nu^2)\frac{1}{n^4}\right]\\
&+\frac{1}{c^6}\Bigg[3\big(i_1(\nu)-\sigma(\nu)\big)\frac{1}{j^5 n} + \frac{45}{2}(7-2\nu)\frac{1}{j^4n^2} - \big(i_5(\nu)-\sigma(\nu)\big)\frac{1}{j^3n^3} - \frac{45}{2}(20-3\nu)\frac{1}{j^2n^4}\\
&+\frac{3}{2}(275-50\nu+4\nu^2)\frac{1}{jn^5} - \frac{1}{64}(6363-805\nu+90\nu^2-5\nu^3)\frac{1}{n^6}\Bigg]\Bigg\},\end{aligned} \tag{4.18}$$

where

$$i_5(\nu) = \frac{303}{4} + \left(\frac{41}{64}\pi^2 - \frac{1427}{12}\right)\nu + \frac{281}{24}\nu^2. \tag{4.19}$$

The results (4.14), (4.16), and (4.18) confirm the 2PN results of [14] and extend them to the 3PN level.

The angular frequencies of the (generic) rosette motion of the binary system are then given by differentiating $\widehat{H}$ with respect to the action variables. Namely,

$$\omega_{\rm radial} = \frac{2\pi}{P} = \frac{1}{GM}\frac{\partial \widehat{H}(n,j,m)}{\partial n}, \tag{4.20}$$

$$\omega_{\rm periastron} = \frac{\Delta\Phi}{P} = \frac{2\pi k}{P} = \frac{1}{GM}\frac{\partial \widehat{H}(n,j,m)}{\partial j}. \tag{4.21}$$

Here, $\omega_{\rm radial}$ is the angular frequency of the radial motion, i.e., the angular frequency of the return to the periastron, while $\omega_{\rm periastron}$ is the average angular frequency with which the major axis advances in space.

It is interesting to note that the ambiguity parameter $\sigma(\nu)$ enters only in two of the six independent combinations of n and j which enter at the 3PN level, cf. Eq. (4.18). We note also that if we consider the fiducial range (3.12) the numerical effect of $\sigma(\nu)$ seems to remain rather small compared to the 'non ambiguous' contribution. Indeed, $\sigma(\nu)$ enters Eqs. (4.12), (4.14), (4.16), and (4.18) only through the differences $i_1(\nu)-\sigma(\nu)$, $i_2(\nu)-\sigma(\nu)$, and $i_5(\nu)-\sigma(\nu)$; $i_1(\nu)$ varies between 38.50 when $\nu=0$, and 29.88 when $\nu=1/4$, $i_2(\nu)$ varies between 52.50 when $\nu=0$, and 36.49 when $\nu=1/4$, while $i_5(\nu)$ varies between 75.75 when $\nu=0$, and 48.33 when $\nu=1/4$. The σ ambiguity therefore has only a limited fractional effect on the coefficients it influences: $\leq 10.0\%$, $\leq 8.2\%$, and $\leq 6.2\%$ for the coefficients influenced through $i_1(\nu)-\sigma(\nu)$, $i_2(\nu)-\sigma(\nu)$, and $i_5(\nu)-\sigma(\nu)$, respectively.

By contrast we wish to emphasize that the use of the approximate ansatz (à la Wilson-Mathews [16]) reducing the spatial metric to being conformally flat affects in a numerically much more drastic way the dynamical invariants. Indeed, the difference starts at the observationally much more significant 2PN order. The Wilson-Mathews truncation of the 2PN Hamiltonian is simply obtained by setting $h_{ij}^{\rm TT}=0$ in the formulas of [10]. It reads (in ADM coordinates)

$$\widehat{H}_{\rm WM}(\mathbf{r},\mathbf{p})=\frac{\mathbf{p}^2}{2}-\frac{1}{r}+\frac{1}{c^2}\left\{\frac{1}{8}(3\nu-1)(\mathbf{p}^2)^2-\frac{1}{2}\left[(3+\nu)\mathbf{p}^2+\nu(\mathbf{n}\cdot\mathbf{p})^2\right]\frac{1}{r}+\frac{1}{2r^2}\right\}$$
$$+\frac{1}{c^4}\left\{\frac{1}{16}\left(1-5\nu+5\nu^2\right)(\mathbf{p}^2)^3+\frac{5}{8}\left(1-4\nu\right)(\mathbf{p}^2)^2\frac{1}{r}\right.$$
$$\left.+\frac{1}{4}\left[(10+19\nu)\mathbf{p}^2-3\nu(\mathbf{n}\cdot\mathbf{p})^2\right]\frac{1}{r^2}-\frac{1}{4}(1+\nu)\frac{1}{r^3}\right\}. \tag{4.22}$$

Rieth [17] has computed (following, as above, the route of Ref. [14]) the invariant functions of $\widehat{H}_{\rm WM}$, Eq. (4.22). They read (see Eqs. (5) and (8) in [17])

$$\frac{P}{2\pi GM}=\frac{1}{(-2E)^{3/2}}\left\{1-\frac{1}{c^2}\frac{1}{4}(15-\nu)\,E+\frac{1}{c^4}\left[\frac{1}{8}(60-18\nu-41\nu^2)\frac{(-2E)^{3/2}}{j}-\frac{15}{32}(7+6\nu-25\nu^2)\,E^2\right]\right\}, \tag{4.23}$$

$$k=\frac{1}{c^2}\frac{3}{j^2}\left\{1+\frac{1}{c^2}\left[\frac{1}{16}(140-54\nu-31\nu^2)\frac{1}{j^2}+\frac{1}{24}(60-18\nu-41\nu^2)\,E\right]\right\}. \tag{4.24}$$

The corresponding Delaunay Hamiltonian reads

$$\widehat{H}_{\rm WM}(n,j,m)=-\frac{1}{2n^2}\left\{1+\frac{1}{c^2}\left[\frac{6}{jn}-\frac{1}{4}(15-\nu)\frac{1}{n^2}\right]\right.$$
$$\left.+\frac{1}{c^4}\left[\frac{1}{8}(140-54\nu-31\nu^2)\frac{1}{j^3n}+\frac{27}{j^2n^2}-\frac{1}{8}(420-42\nu-41\nu^2)\frac{1}{jn^3}+\frac{5}{8}(29-3\nu-3\nu^2)\frac{1}{n^4}\right]\right\}. \tag{4.25}$$

When comparing Eqs. (4.23)–(4.25) to the 2PN-accurate versions of Eqs. (4.14), (4.16), and (4.18) we see that the maximum fractional difference in the 2PN-level coefficients (between the exact $\widehat{H}_{\rm 2PN}$ and the Wilson-Mathews truncation $\widehat{H}_{\rm WM}$) is about 23% (for $\nu=1/4$, and the coefficient of E^2 on the R.H.S. of Eq. (4.23)). 2PN-level effects are crucial in determining important observables, such as the location of the Last Stable Orbit (as discussed, e.g., in Refs. [4,18], and in our follow up work [5]), and are numerically more important than 3PN-level effects (even near the Last Stable Orbit the PN expansion parameter $v^2/c^2\sim 1/6$ is still smallish). Therefore we consider that the Wilson-Mathews truncation is, *a priori*, unacceptably inaccurate. We shall come back below, and in Ref. [5], to the more delicate problem of judging whether the 3PN-level uncertainty (3.12) on σ is practically acceptable or not.

V. DYNAMICAL INVARIANTS FOR THE 3PN CIRCULAR MOTION

In the previous section we considered the invariant functions associated to generic (bound) 3PN orbits ($E<0$). These orbits correspond to a doubly periodic rosette motion. The case of circular orbits, though quite special from a general point of view, plays a physically very important role and deserves a dedicated study. Circular orbits represent the degenerate limit where the integration range $[r_{\rm min},r_{\rm max}]$ in Eq. (4.5) shrinks to a point. [In invariant terms, circular orbits are characterized by the fact that the motion becomes simply periodic, instead of doubly periodic.] Technically they are therfore characterized by setting the radial action i_r, Eq. (4.5), to zero. In other words, the reduced 'principal quantum number' $n=i_r+j$ should be equalled to j. Using Eq. (4.18) this gives the following link, between energy and angular momentum, characterizing circular orbits:

$$E_{\rm circ}=-\frac{1}{2j^2}\left[1+\frac{1}{c^2}\frac{1}{4}(9+\nu)\frac{1}{j^2}+\frac{1}{c^4}\frac{1}{8}(81-7\nu+\nu^2)\frac{1}{j^4}+\frac{1}{c^6}2\big(o_1(\nu)-\sigma(\nu)\big)\frac{1}{j^6}\right], \tag{5.1}$$

where

$$o_1(\nu) = \frac{3861}{128} + \frac{1}{64}\left(41\pi^2 - \frac{8833}{6}\right)\nu + \frac{313}{192}\nu^2 + \frac{5}{128}\nu^3. \tag{5.2}$$

Note that, evidently, it was not needed to derive the full Delaunay Hamiltonian (4.18) to get the result (5.1). It would have been sufficient to impose that the effective radial potential $R(r, E, j)$, Eq. (4.4), have a double zero, i.e. that $\partial R/\partial r = 0 = \partial^2 R/\partial r^2$, or equivalently that the Hamiltonian $\widehat{H}(\mathbf{r}, \mathbf{p})$ (reduced to circular orbits by setting $\mathbf{n}\cdot\mathbf{p} = 0$, $\mathbf{p}^2 = j^2/r^2$) has a minimum when considered as a function of r for fixed j. Let us also give (though it is not an invariant function) the expression of the coordinate radius r (which is the shifted r' of Eq. (2.23)) in function of j

$$r = j^2\left\{1 - \frac{1}{c^2}\frac{4}{j^2} - \frac{1}{c^4}\frac{1}{8}(74 - 43\nu)\frac{1}{j^4} - \frac{1}{c^6}\left[55 + \left(\frac{163}{64}\pi^2 - \frac{1655}{16} - 4\omega_{\rm static}\right)\nu + \left(\frac{61}{6} - 5\omega_{\rm kinetic}\right)\nu^2\right]\frac{1}{j^6}\right\}. \tag{5.3}$$

An important observational quantity is the angular frequency of circular orbits, $\omega_{\rm circ}$. Let us first recall that $\omega_{\rm circ}$ differs from the above considered periastron-to-periastron or radial frequency $\omega_{\rm radial}$, Eq. (4.20). In fact, because the frequency $\omega_{\rm radial}$ measures the frequency in the 'rotating frame' of an orbit which precesses in space with the frequency $\omega_{\rm periastron}$ (4.21), it is easy to see that

$$\omega_{\rm circ} = \omega_{\rm radial} + \omega_{\rm periastron} = 2\pi\frac{1+k}{P}. \tag{5.4}$$

Remembering that $n = j$ along circular orbits we see from Eq. (4.20) that

$$\omega_{\rm circ} = \frac{1}{GM}\frac{dE_{\rm circ}}{dj}, \tag{5.5}$$

which corresponds to the usual link $d\mathcal{E} = \omega_{\rm circ} dJ$ between the (unreduced) total energy $\mathcal{E} = Mc^2 + \mathcal{E}^{\rm NR}$ and the total angular momentum $J = \mu GMj$. As usual, it is convenient to introduce the (coordinate-invariant) dimensionless variable

$$x \equiv \left(\frac{GM\omega_{\rm circ}}{c^3}\right)^{2/3}. \tag{5.6}$$

In the following, we shall set $c = 1$ to simplify the formulas. Inserting Eq. (5.1) into Eq. (5.5) gives the link

$$GM\omega_{\rm circ} \equiv x^{3/2} = \frac{1}{j^3}\left[1 + \frac{1}{2}(9+\nu)\frac{1}{j^2} + \frac{3}{8}(81 - 7\nu + \nu^2)\frac{1}{j^4} + 8\big(o_1(\nu) - \sigma(\nu)\big)\frac{1}{j^6}\right]. \tag{5.7}$$

By inverting this relation one gets j as a function of x:

$$j_{\rm circ} = x^{-1/2}\left[1 + \frac{1}{6}(9+\nu)x + \frac{1}{24}(81 - 57\nu + \nu^2)x^2 + \frac{8}{3}\big(o_2(\nu) - \sigma(\nu)\big)x^3\right], \tag{5.8}$$

where

$$o_2(\nu) = \frac{405}{128} + \frac{1}{64}\left(41\pi^2 - \frac{6889}{6}\right)\nu + \frac{421}{192}\nu^2 + \frac{7}{3456}\nu^3. \tag{5.9}$$

At this point it is useful to consider the test-mass limit ($\nu \to 0$). Indeed, in this limit, i.e. in the case of a test particle m_2 moving, on a circular orbit, in a Schwarzschild background of mass m_1 (with $m_2 \ll m_1$), we have the relations (see, e.g., Eqs. (5.19)–(5.22) in [18])

$$j = \frac{1}{\sqrt{x(1-3x)}}, \tag{5.10a}$$

$$\frac{1}{j^2} = x(1-3x). \tag{5.10b}$$

Here the variable x is defined as in Eq. (5.6), with $M = m_1 + m_2$, and $j \equiv J/(\mu GM) = J/(Gm_1m_2)$, where J is the total angular momentum of the system (which is entirely carried by the test particle). [At this stage we could equivalently consider that M is the mass of the black hole and $\mu \equiv m_1 m_2/M$ the mass of the test particle.] The test mass result (5.10b) suggests to focus on the function $j^{-2}(x)$, which, from Eq. (5.8), is given, when $\nu \neq 0$, by

$$\frac{1}{j_{\rm circ}^2} = x\left[1 - \frac{1}{3}(9+\nu)x + \frac{25}{4}\nu x^2 - \frac{16}{3}\big(o_3(\nu) - \sigma(\nu)\big)x^3\right], \tag{5.11}$$

where

$$o_3(\nu) = \frac{1}{64}\left(41\pi^2 - \frac{5269}{6}\right)\nu + \frac{511}{192}\nu^2 - \frac{1}{432}\nu^3. \tag{5.12}$$

Let us also consider the energy for circular orbits. By inserting Eq. (5.11) into Eq. (5.1) we get

$$E_{\rm circ} \equiv \frac{\mathcal{E}^{\rm total} - M}{\mu} = -\frac{1}{2}x\left[1 - \frac{1}{12}(9+\nu)x - \frac{1}{24}(81 - 57\nu + \nu^2)x^2 - \frac{10}{3}\big(o_2(\nu) - \sigma(\nu)\big)x^3\right], \tag{5.13}$$

where $o_2(\nu)$ is given in Eq. (5.9). It is easily verified that Eqs. (5.8) and (5.13) satisfy (at the 3PN accuracy) the exact identity following from Eq. (5.5)

$$\frac{dE_{\rm circ}}{dx} = x^{3/2}\frac{dj_{\rm circ}}{dx}. \tag{5.14}$$

When comparing Eq. (5.13) with the test-mass limit, there is a problem of definition of the best energy variable to use in a binary system. Indeed, if we consider a test mass of mass m_2 moving around a Schwarzschild black hole of mass m_1, the total energy of the system reads

$$\mathcal{E}^{\rm total} = m_1 + \mathcal{E}_2^{\rm TM} = m_1 - k_\mu p_2^\mu \simeq m_1 - \frac{p_{1\mu}p_2^\mu}{m_1}, \tag{5.15}$$

where p_2^μ is the 4-momentum of the test mass m_2, and $\mathcal{E}_2^{\rm TM} = -k_\mu p_2^\mu$ is the conserved relativistic energy. Here, k^μ is the time-translation Killing vector which is (approximately) $k^\mu = p_1^\mu/m_1$, where p_1^μ is the 4-momentum of the large mass. Eq. (5.15), and the known results for circular motion in Schwarzschild (still with $\mu \equiv m_1 m_2/(m_1+m_2) \simeq m_2$ modulo $\mathcal{O}(\nu)$), yield

$$E = \frac{\mathcal{E}^{\rm total} - m_1 - m_2}{\mu} \simeq \frac{\mathcal{E}_2^{\rm TM} - m_2}{m_2} = \frac{1-2x}{\sqrt{1-3x}} - 1. \tag{5.16}$$

As emphasized in Ref. [4] the expression (5.15) is very asymmetric with respect to the labels 1 and 2. It seems much better to consider the Mandelstam invariant $s = (\mathcal{E}^{\rm total})^2 = -(p_1+p_2)^2 = m_1^2 + m_2^2 - 2p_1\cdot p_2$ and therefore the combination

$$\frac{(\mathcal{E}^{\rm total})^2 - m_1^2 - m_2^2}{2m_1m_2} = -\frac{p_1\cdot p_2}{m_1m_2} \simeq \frac{\mathcal{E}_2^{\rm TM}}{m_2} = \frac{1-2x}{\sqrt{1-3x}}. \tag{5.17}$$

This consideration, and the fact that the energy combination defined by the left-hand side of (5.17) still exhibits a branch cut singularity in the complex x-plane, motivated Ref. [4] to introduce a new invariant energy function e, defined by

$$1 + e \equiv \left(\frac{(\mathcal{E}^{\rm total})^2 - m_1^2 - m_2^2}{2m_1m_2}\right)^2. \tag{5.18}$$

In terms of $E \equiv \widehat{\mathcal{E}}^{\rm NR} \equiv \mathcal{E}^{\rm NR}/\mu \equiv (\mathcal{E}^{\rm total} - M)/\mu$, the new energy function e reads

$$e = \left(1 + E + \frac{\nu}{2}E^2\right)^2 - 1 = 2E + (1+\nu)E^2 + \nu E^3 + \frac{\nu^2}{4}E^4. \tag{5.19}$$

Inserting Eq. (5.13) into Eq. (5.19) yields (at 3PN)

$$e(x,\nu) = -x\left[1 - \frac{1}{3}(3+\nu)x - \frac{1}{12}(36 - 35\nu)x^2 - \frac{10}{3}\big(o_4(\nu) - \sigma(\nu)\big)x^3\right], \tag{5.20}$$

where

$$o_4(\nu) = \frac{27}{10} + \frac{1}{16}\left(\frac{41}{4}\pi^2 - \frac{4309}{15}\right)\nu + \frac{77}{30}\nu^2 - \frac{1}{270}\nu^3. \tag{5.21}$$

From Eq. (5.17) the test-mass limit of this function takes the simple (meromorphic) form

$$e(x,0) = -x\frac{1-4x}{1-3x}. \tag{5.22}$$

For completeness, let us note that the test-mass limit of the invariant link between energy and angular momentum, Eq. (5.1), reads

$$1 + E = \frac{\sqrt{2}}{3}\frac{2+\sqrt{\Delta(j)}}{\sqrt{1+\sqrt{\Delta(j)}}}; \quad \Delta(j) \equiv 1 - \frac{12}{j^2}. \tag{5.23}$$

Actually, the result (5.23) holds only along the sequence of *stable* circular orbits (of Schwarzschild radius $R > 6GM$, i.e. for a frequency parameter $x = GM/R < 1/6$). When $x > 1/6$ (but $x < 1/3$), i.e. for unstable circular orbits $\sqrt{\Delta}$ should be replaced by $-\sqrt{\Delta}$ in (5.23). This corresponds to the fact that the curve $E = E(j)$ has a cusp at the Last Stable Orbit.

To complete our list of exact results in the test-mass limit, let us also note that the periastron parameter $1 + k = \Phi/(2\pi)$ is given, in the limit of circular orbits, by [14,19]

$$1 + k = \left(1 - \frac{12}{j^2}\right)^{-1/4}. \tag{5.24}$$

Inserting Eq. (5.1) into Eq. (4.24) we get, for circular orbits,

$$k_{\rm circ} = \frac{3}{j^2} + \frac{1}{2}(45 - 12\nu)\frac{1}{j^4} + 6\big(o_5(\nu) - \sigma(\nu)\big)\frac{1}{j^6}, \tag{5.25}$$

where

$$o_5(\nu) = \frac{135}{4} + \left(\frac{41}{64}\pi^2 - \frac{101}{3}\right)\nu + \frac{53}{24}\nu^2. \tag{5.26}$$

From Eq. (5.25) follows that

$$(1 + k_{\rm circ})^{-4} = 1 - \frac{12}{j^2} + 24\nu\frac{1}{j^4} - 24\big(o_6(\nu) - \sigma(\nu)\big)\frac{1}{j^6}, \tag{5.27}$$

where

$$o_6(\nu) = \left(\frac{41}{64}\pi^2 - \frac{56}{3}\right)\nu + \frac{53}{24}\nu^2. \tag{5.28}$$

We will use in a further work [5] the various invariant functions computed above, at the 3PN level, to discuss the observable quantities associated to the Last Stable (circular) Orbit of a binary system. For the time being, we shall only remark that, contrary to what happened above in the dynamical invariants for generic orbits, one anticipates that the incomplete knowledge of the ambiguity parameter $\sigma(\nu)$ might be much more serious in the dynamics of circular orbits. Indeed, if we consider for instance the function $j^{-2}(x)$, Eq. (5.11), we see that $\sigma(\nu)$ modifies the coefficient of x^3 through the difference $o_3(\nu) - \sigma(\nu)$; $o_3(\nu)$ vanishes when $\nu = 0$ and decreases monotonically with ν, taking the value -1.683 when $\nu = 1/4$. Therefore the addition of $\sigma(\nu)$, within the range (3.12), can modify a lot the coefficient of x^3 in $j^{-2}(x)$. Similarly, in the case of the original energy function $E(x)$, Eq. (5.13), $\sigma(\nu)$ is subtracted from the coefficient $o_2(\nu)$ which decreases monotonically with ν and varies between $o_2(0) = 3.164$ and $o_2(1/4) = 0.397$. This issue will be discussed in detail in [5].

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APPENDIX A: AMBIGUITIES IN THE 3PN ADM TWO-BODY POINT-MASS HAMILTONIAN

In this appendix we recalculate the 3PN ADM two-body point-mass Hamiltonian given in Ref. [2] and we discuss the plausible range of the ambiguity parameter σ, Eq. (3.8). [We use here the notation of [2], notably $16\pi G = 1$.] The motivation for recalculating the Hamiltonian is three-fold: (i) We want to avoid using explicit solutions of some Poisson equations with complicated (and singular) source terms (it was shown in Ref. [13] that it may not be possible to obtain unique solutions to these equations). (ii) Before applying any regularization procedure we want to represent the Hamiltonian as a volume integral with an integrand which diverges locally as weakly as possible (thus absorbing stronger divergent terms into surface integrals). (iii) We wish to eliminate all 'contact' terms (Dirac delta functions) in the Hamiltonian, so that *only one* regularization procedure is needed (the one used to regularize the volume integral giving the Hamiltonian).

Our starting point is the 3PN Hamiltonian $\widetilde{H}_{3\text{PN}}$ as given by Eqs. (54)–(60) of Ref. [2]. In the first step we eliminate from $\widetilde{H}_{31}$ (given by Eq. (55) of [2]) the function $\phi_{(8)1}$ by integrating by parts[7]: $\phi_{(8)1}\sum_a m_a\delta_a = -\phi_{(8)1}\left(\Delta\phi_{(2)}\right) = -\left(\Delta\phi_{(8)1}\right)\phi_{(2)}+$ exact divergence. To do this we use the equation (see Eqs. (A11) and (A12) in [2])

$$\Delta\phi_{(8)1} = \sum_a \left\{ \frac{1}{512}\phi_{(2)}^3 - \frac{1}{32}\phi_{(2)}\phi_{(4)} + \frac{1}{8}\phi_{(6)} + \left(\frac{5}{16}\phi_{(4)} - \frac{15}{128}\phi_{(2)}^2\right)\frac{\mathbf{p}_a^2}{m_a^2} \right.$$
$$\left. - \frac{9}{64}\phi_{(2)}\frac{(\mathbf{p}_a^2)^2}{m_a^4} - \frac{1}{16}\frac{(\mathbf{p}_a^2)^3}{m_a^6} + \frac{1}{2}\frac{p_{ai}p_{aj}}{m_a^2}h^{\rm TT}_{(4)ij} \right\} m_a\delta_a + \frac{1}{2}\phi_{(4),ij}h^{\rm TT}_{(4)ij} + \frac{1}{2}\Delta\left\{\left(h^{\rm TT}_{(4)ij}\right)^2\right\}. \tag{A1}$$

When performing an integration by parts we always check that the exact-divergence terms fall off at infinity faster than $1/r^4$, so that (formally) they do not contribute to the Hamiltonian. In the next step we split the function $\phi_{(6)}$ into three parts (see Eq. (A4) in [2])

$$\phi_{(6)} = \phi_{(6)1} + \phi_{(6)2} + \phi_{(6)3}, \tag{A2}$$

and we eliminate the functions $\phi_{(6)2}$ and $\phi_{(6)3}$. To perform this we use again integration by parts and equations (see Eqs. (A6) and (A7) in [2])

$$\Delta\phi_{(6)2} = -\left(\widetilde{\pi}^{ij}_{(3)}\right)^2, \tag{A3}$$

$$\Delta\phi_{(6)3} = \frac{1}{2}\phi_{(2),ij}h^{\rm TT}_{(4)ij}. \tag{A4}$$

The elimination of the functions $\phi_{(8)1}$, $\phi_{(6)2}$, and $\phi_{(6)3}$ means that the goal indicated in the item (i) at the beginning of this appendix is achieved; the Hamiltonian depends only on the three lowest-order solutions of the Hamiltonian constraint: $\phi_{(2)}$, $\phi_{(4)}$, and $\phi_{(6)1}$. These three functions are not influenced by the possible ambiguities in solving the Hamiltonian constraint discussed in Ref. [13]. To achieve the goals of items (ii) and (iii) one must perform many integration by parts and employ several times the equations fulfilled by the functions $\phi_{(2)}$, $\phi_{(4)}$, and $\phi_{(6)1}$, which read (see Eqs. (15), (16), and (A5) in [2])

$$\Delta\phi_{(2)} = -\sum_a m_a\delta_a, \tag{A5}$$

$$\Delta\phi_{(4)} = \sum_a \left(\frac{1}{8}\phi_{(2)} - \frac{1}{2}\frac{\mathbf{p}_a^2}{m_a^2}\right) m_a\delta_a, \tag{A6}$$

$$\Delta\phi_{(6)1} = \sum_a \left(-\frac{1}{64}\phi_{(2)}^2 + \frac{1}{8}\phi_{(4)} + \frac{5}{16}\phi_{(2)}\frac{\mathbf{p}_a^2}{m_a^2} + \frac{1}{8}\frac{(\mathbf{p}_a^2)^2}{m_a^4}\right) m_a\delta_a. \tag{A7}$$

Finally, we are able to put the 3PN two-body point-mass ADM Hamiltonian in the following form (dropping many surface terms, after checking that they fall off fast enough at infinity not to contribute to the Hamiltonian)

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[7] In this appendix we abbreviate $\delta(\mathbf{x} - \mathbf{x}_a)$ by δ_a.

$$\widetilde{H}_{3\mathrm{PN}} = -\frac{5}{128}\sum_a \frac{(\mathbf{p}_a^2)^4}{m_a^7} + \int d^3x\,(h_1 + h_2 + h_3), \tag{A8}$$

where

$$h_1 = \frac{1}{8}\left(\frac{5}{16}\phi_{(2)}^3 - \frac{11}{4}\phi_{(2)}\phi_{(4)} + \phi_{(6)1}\right)_{,i} S_{(4),i} + \frac{1}{16}\left(\frac{13}{8}\phi_{(2)}^2 - 3\phi_{(4)}\right)_{,i} S_{(4),i} + \frac{7}{64}\phi_{(2),i}S_{(8),i} - \frac{1}{4}h^{\mathrm{TT}}_{(4)ij,k}S_{(6)ij,k}$$
$$+ \left(\frac{1}{8}S_{(4)} - \frac{5}{4}\phi_{(4)}\right)\left(\tilde{\pi}^{ij}_{(3)}\right)^2 + \left(\frac{1}{16}S_{(4),j} - \frac{3}{8}\phi_{(4),j}\right)\phi_{(2),i}h^{\mathrm{TT}}_{(4)ij} - \left(\left(\phi_{(2)}\tilde{\pi}^{ij}_{(3)}\right)^{\mathrm{TT}}\right)^2$$
$$-\frac{1}{4}\left(\dot{h}^{\mathrm{TT}}_{(4)ij}\right)^2 - \frac{1}{2}\dot{h}^{\mathrm{TT}}_{(4)ij}\left(\phi_{(2)}\tilde{\pi}^{ij}_{(3)}\right)^{\mathrm{TT}}, \tag{A9a}$$

$$h_2 = \frac{1}{32}\left[\left(\phi_{(2)}^2\right)_{,i}\phi_{(6)1,i} + 3\left(\phi_{(2)}\phi_{(4)}\right)_{,i}\phi_{(4),i} + 2\left(\phi_{(4)}^2\right)_{,i}\phi_{(2),i}\right], \tag{A9b}$$

$$h_3 = \frac{35}{64}\phi_{(2)}^2\left(\tilde{\pi}^{ij}_{(3)}\right)^2 + 2\tilde{\pi}^{ik}_{(3)}\tilde{\pi}^{jk}_{(3)}h^{\mathrm{TT}}_{(4)ij} - 2\left(2\pi^i_{(3)} + \Delta^{-1}\pi^l_{(3),il}\right)_{,k}\tilde{\pi}^{jk}_{(3)}h^{\mathrm{TT}}_{(4)ij}$$
$$+ \left(2\pi^i_{(3)} + \Delta^{-1}\pi^l_{(3),il}\right)\left(2\pi^k_{(3)} + \Delta^{-1}\pi^m_{(3),km}\right)_{,j}h^{\mathrm{TT}}_{(4)ij,k}$$
$$+\frac{5}{64}\phi_{(2)}\phi_{(2),i}\phi_{(2),j}h^{\mathrm{TT}}_{(4)ij} - \left(\frac{1}{4}h^{\mathrm{TT}}_{(4)ij} + \frac{5}{8}S_{(4)ij}\right)_{,k}\left(\phi_{(2)}h^{\mathrm{TT}}_{(4)ij}\right)_{,k}. \tag{A9c}$$

In Eqs. (A9a)-(A9c) the following notation was introduced

$$S_{(4)} \equiv -\frac{1}{4\pi}\sum_a \frac{\mathbf{p}_a^2}{m_a r_a}, \tag{A10a}$$

$$S_{(4)ij} \equiv -\frac{1}{4\pi}\sum_a \frac{p_{ai}p_{aj}}{m_a r_a}, \tag{A10b}$$

$$S_{(6)} \equiv -\frac{1}{4\pi}\sum_a \frac{(\mathbf{p}_a^2)^2}{m_a^3 r_a}, \tag{A10c}$$

$$S_{(6)ij} \equiv -\frac{1}{4\pi}\sum_a \frac{\mathbf{p}_a^2 p_{ai}p_{aj}}{m_a^3 r_a}, \tag{A10d}$$

$$S_{(8)} \equiv -\frac{1}{4\pi}\sum_a \frac{(\mathbf{p}_a^2)^3}{m_a^5 r_a}. \tag{A10e}$$

We have not found any ambiguity connected with the regularization of the divergent integrals contained in the first part h_1 of the Hamiltonian (see below for details). Regularization of the h_2 part contributes only to the static ambiguity, and regularization of the h_3 part contributes only to the kinetic ambiguity. The static part of the 3PN Hamiltonian (discussed in detail in Ref. [13]; see footnote 6 in the present paper) is equal to $\int d^3x\, h_2$.

We regularize all the divergent integrals involved in the Hamiltonian given by Eqs. (A8)–(A9) by means of the Riesz-formula-based regularization technique described in Appendix B 2 of [2] and rediscussed in Sec. III of the present paper. The final result, after eliminating the time derivatives of the particle positions and momenta by using the Newtonian equations of motion, Eq. (3.1), is given in Eq. (3.6).

To investigate the lack of uniqueness of the regularization method we have used the following procedure. To many individual terms in Eqs. (A9) one can associate exact divergences which must be added to these terms to replace them by some of their integration-by-parts equivalents. E.g., with the first term in Eq. (A9a) one can associate two exact divergences, $-\frac{5}{128}[(\phi_{(2)}^3)_{,i}S_{(4)}]_{,i}$ and $-\frac{5}{128}[\phi_{(2)}^3 S_{(4),i}]_{,i}$. The result of the regularization method is stable against integration by parts only if the regularized value of the integral of any of these exact divergences is zero.

With h_1, Eq. (A9a), one can associate the following 18 exact divergences

$$-\frac{5}{128}\left[\left(\phi_{(2)}^3\right)_{,i}S_{(4)}\right]_{,i},\ -\frac{5}{128}\left[\phi_{(2)}^3 S_{(4),i}\right]_{,i},\ \frac{11}{32}\left[\left(\phi_{(2)}\phi_{(4)}\right)_{,i}S_{(4)}\right]_{,i},\ \frac{11}{32}\left[\phi_{(2)}\phi_{(4)}S_{(4),i}\right]_{,i},$$

$$-\frac{1}{8}\left[\phi_{(6)1,i}S_{(4)}\right]_{,i},\ -\frac{1}{8}\left[\phi_{(6)1}S_{(4),i}\right]_{,i},\ -\frac{13}{128}\left[\left(\phi_{(2)}^2\right)_{,i}S_{(6)}\right]_{,i},\ -\frac{13}{128}\left[\phi_{(2)}^2 S_{(6),i}\right]_{,i},$$

$$\frac{3}{16}\left[\phi_{(4),i}S_{(6)}\right]_{,i},\ \frac{3}{16}\left[\phi_{(4)}S_{(6),i}\right]_{,i},\ -\frac{7}{64}\left[\phi_{(2),i}S_{(8)}\right]_{,i},\ -\frac{7}{64}\left[\phi_{(2)}S_{(8),i}\right]_{,i},$$

$$\frac{1}{4}\left[h^{\rm TT}_{(4)ij,k}S_{(6)ij}\right]_{,k},\ \frac{1}{4}\left[h^{\rm TT}_{(4)ij}S_{(6)ij,k}\right]_{,k},\ \frac{3}{8}\left[\phi_{(2),i}\phi_{(4)}h^{\rm TT}_{(4)ij}\right]_{,j},\ \frac{3}{8}\left[\phi_{(2)}\phi_{(4),i}h^{\rm TT}_{(4)ij}\right]_{,j},$$

$$-\frac{1}{16}\left[\phi_{(2),i}S_{(4)}h^{\rm TT}_{(4)ij}\right]_{,j},\ -\frac{1}{16}\left[\phi_{(2)}S_{(4),i}h^{\rm TT}_{(4)ij}\right]_{,j}. \tag{A11}$$

The question now is whether, when explicitly computed (and regularized) by the method we are going to recall, the integrals of the exact divergences in the list (A11) vanish or not. The explicit method of regularized-integration we use is the following: First, we explicitly perform the differentiations present in the divergences using, if necessary, the distributional rule of differentiation of homogeneous functions described in Appendix B 4 of [2] (cf. the example given there). Note that we always use Leibniz's rule when differentiating products of functions, the distributional rule is used only for individual functions (by which we understand the functions explicitly entering Eqs. (A9): $\phi_{(2)}$, $\phi_{(4)}$, $\phi_{(6)1}$, $S_{(4)}$, ...; it implies that in computing the new reference Hamiltonian given by Eqs. (A9) we have not used the distributional rule). E.g., we compute $\left(\phi_{(2)}^2\phi_{(2),j}\right)_{,i}$ in two steps: (i) using Leibniz's rule one gets $\left(\phi_{(2)}^2\phi_{(2),j}\right)_{,i} = 2\phi_{(2)}\phi_{(2),i}\phi_{(2),j} + \phi_{(2)}^2\phi_{(2),ij}$, (ii) the distributional rule is applied only to $\phi_{(2),ij}$. After this, a typical integral consists of two parts: without and with Dirac deltas. The first part is computed by means of the Riesz-formula-based regularization technique, while, for the second part, we have used the Hadamard-partie-finie regularization described in Appendix B 1 of [2]. In the second case we have also investigated the stability of the result against 'threading' the partie finie (Pf) over a product of functions, i.e., we have checked whether

$$\mathrm{Pf}(fg) = \mathrm{Pf}(f)\,\mathrm{Pf}(g). \tag{A12}$$

For all divergences in (A11) the final result of these explicit computations is zero (regardless which side of Eq. (A12) is employed in the contact terms).

With h_2, Eq. (A9b), one can similarly associate the following six integrals of exact divergences

$$\Delta_{21} \equiv -\frac{1}{32}\int d^3x\left[\phi_{(2)}^2\phi_{(6)1,i}\right]_{,i}, \tag{A13a}$$

$$\Delta_{22} \equiv -\frac{1}{32}\int d^3x\left[\left(\phi_{(2)}^2\right)_{,i}\phi_{(6)1}\right]_{,i}, \tag{A13b}$$

$$\Delta_{23} \equiv -\frac{3}{32}\int d^3x\left[\left(\phi_{(2)}\phi_{(4)}\right)_{,i}\phi_{(4)}\right]_{,i}, \tag{A13c}$$

$$\Delta_{24} \equiv -\frac{3}{32}\int d^3x\left[\phi_{(2)}\phi_{(4)}\phi_{(4),i}\right]_{,i}, \tag{A13d}$$

$$\Delta_{25} \equiv -\frac{1}{16}\int d^3x\left[\left(\phi_{(4)}^2\right)_{,i}\phi_{(2)}\right]_{,i}, \tag{A13e}$$

$$\Delta_{26} \equiv -\frac{1}{16}\int d^3x\left[\phi_{(4)}^2\phi_{(2),i}\right]_{,i}. \tag{A13f}$$

Below we denote by primes the result of regularizing with the use of the left-hand side of Eq. (A12) (for these parts of the integrands which are proportional to Dirac deltas), and by double primes the result obtained when using the right-hand side of Eq. (A12). With this notation, the regularized values of the integrals in (A13) read

$$\Delta'_{21} = \frac{1}{4}\frac{\nu}{r^4}, \ \Delta''_{21} = 0, \tag{A14a}$$

$$\Delta'_{22} = \Delta'_{23} = \Delta'_{24} = \Delta'_{25} = \Delta'_{26} = 0, \tag{A14b}$$

$$\Delta''_{22} = \Delta''_{23} = \Delta''_{24} = \Delta''_{25} = \Delta''_{26} = 0. \tag{A14c}$$

With h_3, Eq. (A9c), we associate eight integrals of exact divergences

$$\Delta_{31} \equiv 2\int d^3x \left[\left(2\pi^i_{(3)} + \Delta^{-1}\pi^l_{(3),il}\right)_{,k} \tilde{\pi}^{jk}_{(3)} h^{\rm TT}_{(4)ij}\right]_{,k}, \tag{A15a}$$

$$\Delta_{32} \equiv -\int d^3x \left[\left(2\pi^i_{(3)} + \Delta^{-1}\pi^l_{(3),il}\right)\left(2\pi^k_{(3)} + \Delta^{-1}\pi^m_{(3),km}\right) h^{\rm TT}_{(4)ij,k}\right]_{,j}, \tag{A15b}$$

$$\Delta_{33} \equiv -\int d^3x \left[\left(2\pi^i_{(3)} + \Delta^{-1}\pi^l_{(3),il}\right)\left(2\pi^k_{(3)} + \Delta^{-1}\pi^m_{(3),km}\right)_{,j} h^{\rm TT}_{(4)ij}\right]_{,k}, \tag{A15c}$$

$$\Delta_{34} \equiv -\frac{5}{128}\int d^3x \left[\phi^2_{(2)}\phi_{(2),j} h^{\rm TT}_{(4)ij}\right]_{,i}, \tag{A15d}$$

$$\Delta_{35} \equiv \frac{1}{4}\int d^3x \left[h^{\rm TT}_{(4)ij}\left(\phi_{(2)} h^{\rm TT}_{(4)ij}\right)_{,k}\right]_{,k}, \tag{A15e}$$

$$\Delta_{36} \equiv \frac{1}{4}\int d^3x \left[\phi_{(2)} h^{\rm TT}_{(4)ij} h^{\rm TT}_{(4)ij,k}\right]_{,k}, \tag{A15f}$$

$$\Delta_{37} \equiv \frac{5}{8}\int d^3x \left[\left(\phi_{(2)} h^{\rm TT}_{(4)ij}\right)_{,k} S_{(4)ij}\right]_{,k}, \tag{A15g}$$

$$\Delta_{38} \equiv \frac{5}{8}\int d^3x \left[\phi_{(2)} h^{\rm TT}_{(4)ij} S_{(4)ij,k}\right]_{,k}. \tag{A15h}$$

The results of the regularized-integration of (A15) read (here $\kappa \equiv \nu^2\left(\mathbf{p}^2 - 3(\mathbf{n}\cdot\mathbf{p})^2\right)/r^3$; note that the exact divergences Δ_{32} and Δ_{34} do not contain contact terms)

$$\Delta'_{31} = \frac{7}{10}\kappa, \quad \Delta''_{31} = -\frac{109}{10}\kappa, \tag{A16a}$$

$$\Delta_{32} = -\frac{11}{30}\kappa, \tag{A16b}$$

$$\Delta'_{33} = -\frac{21}{10}\kappa, \quad \Delta''_{33} = \frac{37}{20}\kappa, \tag{A16c}$$

$$\Delta_{34} = -\frac{1}{2}\kappa, \tag{A16d}$$

$$\Delta'_{35} = \frac{32}{25}\kappa, \quad \Delta''_{35} = -\frac{21}{10}\kappa, \tag{A16e}$$

$$\Delta'_{36} = \frac{32}{25}\kappa, \quad \Delta''_{36} = 0, \tag{A16f}$$

$$\Delta'_{37} = -8\kappa, \quad \Delta''_{37} = 0, \tag{A16g}$$

$$\Delta'_{38} = 0, \quad \Delta''_{38} = 8\kappa. \tag{A16h}$$

From Eqs. (A14) and (A16) follows that only one out of the 32 exact divergences considered above, $\Delta_{21} = \nu/(4r^4)$, is connected to the static ambiguity parameter $\omega_{\rm static}$, whereas eight exact divergences Δ_{31}–Δ_{38} 'contribute' to the kinetic ambiguity parameter $\omega_{\rm kinetic}$: their regularized values are between -10.9κ and $+8\kappa$.

We are not confident that the so-found relatively small contribution ($\pm 1/4$) to $\omega_{\rm static}$ is indicative of a smaller ambiguity in $\omega_{\rm static}$ than in $\omega_{\rm kinetic}$. Therefore, we used also another (more primitive, but hopefully more robust) way of estimating the plausible values of the ambiguity parameters $\omega_{\rm static}$ and $\omega_{\rm kinetic}$. We simply looked at the values of all the numerical coefficients in the final 3PN Hamiltonian, Eq. (3.6). The Hamiltonian has 27 numerical coefficients, entering as factors of the different monomials made of powers of $\mathbf{p}^2$, $(\mathbf{n}\cdot\mathbf{p})^2$, $1/r$, and ν. Out of them only three are influenced by ambiguities (the coefficients of $\nu^2\mathbf{p}^2/r^3$, $\nu^2(\mathbf{n}\cdot\mathbf{p})^2/r^3$, and ν/r^4). The numerical values of the unambiguous coefficients range between $\pi^2/64 - 335/48 \approx -6.825$ ($\nu\,\mathbf{p}^2/r^3$) and $17/2 = 8.5$ ($\nu(\mathbf{p}^2)^2/r^2$), whereas the ambiguous coefficients in the reference Hamiltonian (3.6) are equal to $-55/12 \approx -4.583$ ($\nu^2\mathbf{p}^2/r^3$), $27/8 = 3.375$ ($\nu^2(\mathbf{n}\cdot\mathbf{p})^2/r^3$), and $109/12 - 21\pi^2/32 \approx 2.606$ (ν/r^4).

As a result of the above discussion we take, as plausible ranges for the ambiguity parameters $\omega_{\rm static}$ and $\omega_{\rm kinetic}$, the ranges

$$-10 \lesssim \omega_{\rm static} \lesssim 10, \quad -10 \lesssim \omega_{\rm kinetic} \lesssim 10. \tag{A17}$$

APPENDIX B: COMPUTATION OF THE RADIAL ACTION INTEGRAL

The explicit form of the coefficients A, B, C, D_i entering the effective radial potential $R(r,E,j)$, Eq. (4.4), reads

$$A = 2E + \frac{1}{c^2}(1-3\nu)\,E^2 - \frac{1}{c^4}(1-4\nu)\nu\,E^3 + \frac{1}{c^6}\frac{5}{4}(1-4\nu)\nu^2\,E^4, \tag{B1a}$$

$$B = 1 + \frac{1}{c^2}(4-\nu)\,E + \frac{1}{c^4}(2-2\nu+\nu^2)\,E^2 + \frac{1}{c^6}(2-\nu)\nu^2\,E^3, \tag{B1b}$$

$$C = -j^2 + \frac{1}{c^2}(6+\nu) + \frac{1}{c^4}15E + \frac{1}{c^6}\frac{1}{6}(45-38\nu-4\nu^2)\,E^2, \tag{B1c}$$

$$D_1^{\rm 1PN} = -\frac{1}{c^2}\nu\,j^2 + \frac{1}{c^4}\left[\frac{1}{2}(17+5\nu+4\nu^2) - (1+\nu)\nu\,Ej^2\right]$$
$$+\frac{1}{c^6}\left\{\frac{1}{8}\left[144+(\pi^2-212)\nu+16(4\omega_{\rm kinetic}-7)\nu^2+16\nu^3\right]E - \frac{1}{2}\nu^2\,E^2j^2\right\}, \tag{B1d}$$

$$D_2^{\rm 2PN} = -\frac{1}{c^4}(1+3\nu)\nu\,j^2 + \frac{1}{c^6}\left\{\frac{1}{48}\left[384+(69\pi^2-1660-96\omega_{\rm static})\nu+4(96\omega_{\rm kinetic}-139)\nu^2+240\nu^3\right]\right.$$
$$\left.+\frac{1}{12}(79+38\nu-72\nu^2)\nu\,Ej^2\right\}, \tag{B1e}$$

$$D_3^{\rm 2PN} = \frac{1}{c^4}\frac{3}{4}\nu^2\,j^2 + \frac{1}{c^6}\left\{\frac{1}{96}\left[140-9\pi^2+8(191-72\omega_{\rm kinetic})\nu-960\nu^2\right]\nu\,j^2 + \frac{9}{4}\nu^3\,Ej^4\right\}, \tag{B1f}$$

$$D_4^{\rm 3PN} = -\frac{1}{c^6}\frac{1}{6}(5+28\nu-30\nu^2)\nu\,j^4, \tag{B1g}$$

$$D_5^{\rm 3PN} = -\frac{1}{c^6}\frac{5}{8}\nu^3\,j^6. \tag{B1h}$$

The PN expansion of the effective radial action integral i_r, Eq. (4.5), can be written (as explained in Sec. IV of the present paper) as a linear combination of the integrals $J_{q,m}$ defined in Eq. (4.10). The only integrals that one needs to compute at 3PN order are $J_{q,m}$ with $0 \le q \le 3$: when $q=0$, $m=0$; when $q=1$, $3\le m\le 7$; when $q=2$, $6\le m\le 8$; and when $q=3$, $m=9$. The explicit results of the integration (performed by the two methods indicated in the text) read

$$J_{0,0} = \frac{B}{\sqrt{-A}} - \sqrt{-C}, \tag{B2a}$$

$$J_{1,3} = \frac{B}{(-C)^{\frac{3}{2}}}, \tag{B2b}$$

$$J_{1,4} = \frac{3B^2 - AC}{2(-C)^{\frac{5}{2}}}, \tag{B2c}$$

$$J_{1,5} = \frac{B(5B^2 - 3AC)}{2(-C)^{\frac{7}{2}}}, \tag{B2d}$$

$$J_{1,6} = \frac{35B^4 - 30AB^2C + 3A^2C^2}{8(-C)^{\frac{9}{2}}}, \tag{B2e}$$

$$J_{1,7} = \frac{B(63B^4 - 70AB^2C + 15A^2C^2)}{8(-C)^{\frac{11}{2}}}, \tag{B2f}$$

$$J_{2,6} = \frac{3(-5B^2 + AC)}{2(-C)^{\frac{7}{2}}}, \tag{B2g}$$

$$J_{2,7} = \frac{5B(-7B^2 + 3AC)}{2(-C)^{\frac{9}{2}}}, \tag{B2h}$$

$$J_{2,8} = \frac{15(-21B^4 + 14AB^2C - A^2C^2)}{8(-C)^{\frac{11}{2}}}, \tag{B2i}$$

$$J_{3,9} = \frac{35B(3B^2 - AC)}{2(-C)^{\frac{11}{2}}}. \tag{B2j}$$

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