

Hamiltonians and canonical coordinates for spinning particles in curved space-time

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The spin-curvature coupling as captured by the so-called Mathisson-Papapetrou-Dixon (MPD) equations is the leading order effect of the finite size of a rapidly rotating compact astrophysical object moving in a curved background. It is also a next-to-leading order effect in the phase of gravitational waves emitted by extreme-mass-ratio inspirals (EMRIs), which are expected to become observable by the LISA space mission. Additionally, exploring the Hamiltonian formalism for spinning bodies is important for the construction of the so-called Effective-One-Body waveform models that should eventually cover all mass ratios.

The MPD equations require supplementary conditions determining the frame in which the moments of the body are computed. We review various choices of these supplementary spin conditions and their properties. Then, we give Hamiltonians either in proper-time or coordinate-time parametrization for the Tulczyjew-Dixon, Mathisson-Pirani, and Kyrian-Semerák conditions. Finally, we also give canonical phase-space coordinates parametrizing the spin tensor. We demonstrate the usefulness of the canonical coordinates for symplectic integration by constructing Poincaré surfaces of section for spinning bodies moving in the equatorial plane in Schwarzschild space-time. We observe the motion to be essentially regular for EMRI-ranges of the spin, but for larger values the Poincaré surfaces of section exhibit the typical structure of a weakly chaotic system. A possible future application of the numerical integration method is the inclusion of spin effects in EMRIs at the precision requirements of LISA.

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1. INTRODUCTION

The detection of black-hole and neutron-star binary inspirals by the aLIGO and aLIGO-Virgo detectors mark the dawn of gravitational-wave astronomy [1–7]. The equations of Einstein gravity are put to test not only by the phenomenon and detection of gravitational waves itself, but also by the precise shape of the detected signal [8]. Furthermore, the analysis of the signal from neutron-star binaries provides precious astrophysical information about their composition [9–11], and the observations of the electromagnetic aftermath is key to the explanation of the origin of the energetically unfavorable heavy elements in our Universe [12, 13].

Upcoming space-based missions such as LISA promise to probe the gravitational-wave spectrum in lower frequencies than terrestrial detectors such as Advanced LIGO and Virgo and, thus, to explore the dynamics of many other types of sources of gravitational radiation [14]. One such particular class of sources are the so-called extreme-mass-ratio inspirals (EMRIs), during which stellar-mass compact objects spiral into massive black holes, which have masses at least five orders of magnitude above the solar mass [15].

Independent of the mass ratio between the components of the system, neither the primary nor the secondary of the binary can be modeled as point particles in an accurate treatment of the inspiral, and effects of the finite size of the bodies must be taken into account. This is clear in the case of binaries of comparable size and mass, but in the case of EMRIs a more careful argumentation must be given.

Let us denote the mass of the primary massive black hole as M and the mass of the secondary stellar-mass object as μ . Then the mass-ratio in EMRIs is $q \equiv \mu/M \sim 10^{-4} - 10^{-7}$ and one can describe the gravitational field of the secondary as a perturbation on top of the gravitational field of the primary. As a result, the secondary is usually described as moving on the original background while being subject to a self-force whose relative size with respect to the Christoffel-connection terms is of the order $\mathcal{O}(q)$ [see 16, 17, for reviews and a complete list of references].

Now consider the effects of the finite size of the secondary. If the secondary is rotating at relativistic speeds, a matter element on its surface will feel a relative acceleration with respect to the center of mass that is proportional to the velocity of the surface v , the radius of the object r , and the local space-time curvature R . Under the assumption of a balance of forces inside the body, this will result in a “spin force” $\sim \mu vrR$ acting on the center of mass. Let us further assume that the binary orbital separation is within a few horizon radii of the primary, and that the secondary is either a maximally spinning black hole, a few-millisecond pulsar, or a few-second pulsar. We then get respectively $vrR \sim 1q/M, 10^{-1}q/M, 10^{-4}q/M$. When we consider that the Christoffel symbols scale as $\sim 1/M$, we see that the relative size of the acceleration caused by the spin force is then $\mathcal{O}(q)$, the same as the gravitational self-force.

The effects of the self-force and the spin force on the orbit will thus both scale as $\mathcal{O}(q)$ and would be essentially impossible to distinguish from a geodesic when using observables

collected over just a few orbital periods. Nevertheless, the orbit will only decay over $\mathcal{O}(1/q)$ cycles and the small deviations amount to secular effects in the phase of the orbit. The final orbital phase ϕ_f can then be schematically written as a sum of contributions of the form [18]

$$\phi_f = \phi_{\text{avg}}^{(1)} \quad \mathcal{O}(q^{-1}) \quad (1)$$

$$+ \phi_{\text{osc}}^{(1)} + \phi_{\text{avg}}^{(2)} + \phi_{\text{spin}} \quad \mathcal{O}(1) \quad (2)$$

$$+ \phi_{\text{osc}}^{(2)} + \phi_{\text{avg}}^{(3)} + \phi_{\text{quad}} \quad \mathcal{O}(q) \quad (3)$$

$$+ \dots \quad \mathcal{O}(q^2), \quad (4)$$

where “avg” and “osc” stand respectively for contributions from the averaged dissipative, and oscillating dissipative and conservative parts of the self-force computed from the metric perturbations of order (n). Then, at the same order as the first-order conservative piece of the self-force appears the contribution of the spin force. Both the $\mathcal{O}(q^{-1})$ and the $\mathcal{O}(1)$ terms must be eventually included if sub-radian precision is to be achieved in the EMRI wave-form modeling.

The $\mathcal{O}(q)$ contributions to the phase then contain the contribution of the next-to-leading effect of the finite size of the secondary, the quadrupolar coupling. In particular, this will include the spin-induced quadrupole that scales as $\sim S^2$ for neutron stars and black holes [19–21], where $S \sim mrv$ is the spin magnitude. Tidal deformation of the body also formally appears in the quadrupole; however, it can be estimated to enter the equations of motion at relative order $\mathcal{O}(q^4)$ [22–24] and it will thus enter the phase only at $\mathcal{O}(q^3)$ for conservative effects and perhaps at $\mathcal{O}(q^2)$ if the dissipative tidal effects contribute to the orbital decay time.

In summary, we see that the spin-curvature coupling considered at least to linear order is an indispensable piece of any EMRI model. However, the spin-curvature coupling also plays an important role in the post-Newtonian (weak-field and slow-motion) description of comparable-mass binaries [25, 26]; the conservative dynamics includes all fourth-order spin-induced effects so far [27]. But still, a wave-form model that encompasses mass ratios from comparable to extreme is highly desirable. This is one goal of the effect-one-body (EOB) model [28–32], being probably the best candidate to succeed in this endeavor. While incorporating all $\mathcal{O}(1)$ self-force effects is progressing [33], one flavor of EOB models already incorporates the test-spin force on a Kerr background to linear order in the test-spin via a Hamiltonian [29, 34], the central piece encoding the conservative dynamics in any EOB model (but see the progress of the other EOB flavor in Refs. [35–38]). In this context, exploring simplified Hamiltonian descriptions of spinning bodies appears to be crucial.

In this paper, we study the Hamiltonian formalism for a spinning particle moving in a given space-time metric. In Section 2 we review the so-called Mathisson-Papapetrou-Dixon (MPD) equations that capture the effects of the spin force on the orbit, and the properties of the equations under various supplementary conditions that are needed to close the equations.

We then proceed to the Hamiltonian formalism in Section 3. We present the Poisson brackets and various sets of variables that can be used during the evolution, and Hamiltonians

for all the usual ‘‘comoving’’ supplementary conditions both in proper-time and coordinate-time parametrizations. Next, in Section 4, we also give a set of canonical coordinates covering the spin tensor, which is useful for the numerical integration of the MPD equations. Finally, in Section 5, we demonstrate the power of the new coordinates and Hamiltonian formalism by numerically studying spinning particles moving in the equatorial plane of a Schwarzschild black hole.

The paper also contains a number of Appendices that provide context to the presented results and details of the derivations mentioned in the main text.

We use the $G = c = 1$ geometrized units and the $(-+++)$ signature of the metric. Our convention for the Riemann tensor $R^\mu_{\nu\alpha\beta}$ is such that $2a_{\mu;[\alpha\beta]} = R^\nu_{\mu\alpha\beta}a_\nu$ for a generic a_μ , or explicitly $R^\mu_{\nu\alpha\beta} = 2\Gamma^\mu_{\rho[\alpha}\Gamma^\rho_{\beta]\nu} - 2\Gamma^\mu_{\nu[\alpha}\Gamma^\rho_{\beta]\rho}$. The anti-symmetrization of a tensor is written as $W_{[\alpha\beta]} = \frac{1}{2}(W_{\alpha\beta} - W_{\beta\alpha})$, while the symmetrization as $W_{(\alpha\beta)} = \frac{1}{2}(W_{\alpha\beta} + W_{\beta\alpha})$. We denote the covariant time derivative by an overdot, $\dot{A}^{\mu\nu\dots} \equiv DA^{\mu\nu\dots}/d\tau \equiv A^{\mu\nu\dots}_{;\delta}\dot{x}^\delta$. $\eta^{\mu\nu}$ with any indices is the Minkowski tensor, and δ^μ_ν denotes the Kronecker delta.

2. MPD EQUATIONS

The equations of motion of massive bodies in a gravitational field is among the most basic topics in Newtonian mechanics, and among the toughest problems in general relativity. Surprisingly, just assuming the covariant conservation of energy-momentum of the body restricts these equations to be of the celebrated MPD form in general relativity. The MPD equations to pole-dipole order read [39–41]

$$\dot{P}^\mu = -\frac{1}{2}R^\mu_{\nu\kappa\lambda}\dot{x}^\nu S^{\kappa\lambda}, \quad (5a)$$

$$\dot{S}^{\kappa\lambda} = P^\kappa\dot{x}^\lambda - P^\lambda\dot{x}^\kappa, \quad (5b)$$

where $x^\mu(\tau)$ is the world-line of some representative centroid from within the rotating body, $S^{\kappa\lambda}$ the spin tensor, and P^μ the momentum (flux of stress-energy) of the body. Here τ is the proper time, $\dot{x}^\mu\dot{x}_\mu = -1$. But it is noteworthy that the MPD equations are invariant under affine reparametrizations of the world-line.

The relation between \dot{x}^ν and P^ν is underdetermined and has to be derived from a supplementary spin condition. A supplementary spin condition is usually given in the form $S^{\mu\nu}V_\nu = 0$, where V_ν is some time-like vector. The physical interpretation of this supplementary condition is that V^ν is the frame in which the momenta of the stress-energy tensor P^μ and $S^{\nu\kappa}$ are computed, and the position of the referential world-line $x^\mu(\tau)$ is then the center of mass of the spinning body in this frame [42].

The MPD equations as stated here do not include the contributions from the quadrupole and higher-order mass moments of the body. They are in fact universal at pole-dipole order, i.e., independent of the internal structure of the body. Amongst other effects and as already mentioned in the Introduction, one expects the rotation to deform the body and thus produce a

structure-dependent quadrupole moment that scales as S^2 ; this holds in particular for rotating black holes and neutron stars. Since we are not including such spin-quadratic terms in the equations either way, it is often meaningful to truncate the formulas at some low order in S .

Some of the identities that are useful independent of the supplementary condition read

$$\dot{x}^{(\mu}\dot{S}^{\nu\kappa)}_{\text{cycl.}} = 0, \quad (6)$$

$$P^\mu = m\dot{x}^\mu + \dot{x}_\gamma\dot{S}^{\gamma\mu}, \quad (7)$$

$$m \equiv -P^\mu\dot{x}^\mu. \quad (8)$$

A number of other useful identities along with a brief historical review of the MPD equations can be found in Ref. [43].

We also define the spin vector s^μ , the spin magnitude S , and a mass-like quantity \mathcal{M} by

$$s^\mu \equiv -\frac{1}{2\sqrt{-V^\alpha V_\alpha}}\epsilon^{\mu\nu\kappa\lambda}V_\nu S_{\kappa\lambda} = -\frac{1}{\sqrt{-V^\alpha V_\alpha}}\star S^{\mu\nu}V_\nu, \quad (9)$$

$$S \equiv \sqrt{\frac{S^{\kappa\lambda}S_{\kappa\lambda}}{2}} = \sqrt{s^\mu s_\mu}, \quad (10)$$

$$\mathcal{M} \equiv \sqrt{-P^\alpha P_\alpha}, \quad (11)$$

where $\star S^{\mu\nu} = \epsilon^{\mu\nu\kappa\lambda}S_{\kappa\lambda}/2$. It should be noted that the definition of s^μ will be different whenever a different supplementary condition is chosen. Now we see that $S^{\kappa\lambda}s_\lambda = 0$ and we can build a projector on the sub-space orthogonal to V_μ, s_ν as

$$h^\mu_\nu = \frac{1}{S^2}S^{\mu\kappa}S_{\nu\kappa} = \left(\delta^\mu_\nu + \frac{V^\mu V_\nu}{(-V^\alpha V_\alpha)} - \frac{s^\mu s_\nu}{S^2}\right). \quad (12)$$

Now, the question is which supplementary spin condition should be adopted to close the system of MPD equations. The best answer that one can give, however, is that virtually any condition is physically viable, at least at the (universal) pole-dipole order. Hence, in the remaining part of this section, we review all commonly proposed classes of supplementary spin conditions.

2.1. The KS condition

Eq. (7) indicates that the momentum is generally linearly independent of the four-velocity. Kyriani and Semerák [44] (KS) asked the question under which supplementary condition is the momentum proportional to the four-velocity, $P^\mu = m\dot{x}^\mu$, and found that this is true when we assume the existence of a time-like vector w_μ such that $S^{\mu\nu}w_\nu = 0$ and $\dot{w}_\nu = 0$. We also conventionally set $w_\alpha w^\alpha = -1$. The MPD equations then simplify into the form

$$P^\mu = m\dot{x}^\mu, \quad (13a)$$

$$\dot{m} = 0, \quad (13b)$$

$$\dot{x}^\mu = -\frac{1}{2m}R^\mu_{\nu\kappa\lambda}\dot{x}^\nu S^{\kappa\lambda}, \quad (13c)$$

$$\dot{S}^{\kappa\lambda} = 0. \quad (13d)$$

This is probably the simplest form of the MPD equations one can acquire and it can in fact be generated by a large set of other supplementary conditions, which is discussed in Appendix A.

In terms of variables that need to be stored and updated during every step of a numerical integration, the system of equations (13) is characterized by a phase space $(x^\mu, \dot{x}^\nu, S^{\kappa\lambda})$. An important point is to realize that once an initial condition with some vanishing direction of the spin tensor is chosen, $S^{\mu\nu}w_\nu|_{\tau=\tau_0} = 0$, the equations of motion (13) will evolve with two vanishing directions (the first one proportional to w^μ , and the second one proportional to s^μ) in a way so that we can always choose for one of them to fulfill $\dot{w}^\mu = 0$. In other words, once the initial condition is set up with a degenerate spin tensor, the set of equations (13) can be evolved at face value without further reference to the auxiliary vector w^μ .

Nevertheless, the equations of motion can also be re-expressed using w_ν and the respective spin vector s_μ as

$$\ddot{x}^\mu = \frac{1}{m} \star R_{\nu\kappa\lambda}^\mu \dot{x}^\nu s^\kappa w^\lambda, \quad (14a)$$

$$\dot{w}^\kappa = \dot{s}^\lambda = 0, \quad (14b)$$

where $\star R_{\mu\nu\kappa\lambda} \equiv R_{\mu\nu\gamma\delta} \epsilon^{\gamma\delta}_{\kappa\lambda} / 2$. In this case the phase space $(x^\mu, \dot{x}^\nu, s^\lambda, w^\kappa)$ consists of the coordinate positions, velocities, the spin vector, and the auxiliary vector w^λ .

2.2. The MP condition

Another supplementary spin condition considered by various authors [39, 45, 46] is $S^{\mu\nu}\dot{x}_\nu = 0$. We will call it the Mathisson-Pirani (MP) spin condition due to the pioneering works using this condition in the context of curved space-time [39, 46]; in the context of flat space-time, it is often called the Frenkel spin condition due to the pioneering work of Frenkel [45]. Under this supplementary condition, the MPD equations are simply the equations (5) with the substitution of the following relation in place of \dot{x}^μ [47]

$$\dot{x}^\mu = \frac{1}{m} P^\nu \left(\delta_\nu^\mu - \frac{1}{S^2} S^{\mu\kappa} S_{\nu\kappa} \right) = P^\nu (\delta_\nu^\mu - h_{\nu}^\mu). \quad (15)$$

Once again, in this representation the phase space needed for numerical evolution is $(x^\mu, P^\nu, S^{\kappa\lambda})$, the same number of variables as for the KS condition.

Another representation of the phase space is through the spin vector and higher order derivatives of the position:

$$\ddot{x}^\mu = f^\mu(x^\nu, \dot{x}^\lambda, \ddot{x}^\kappa, s^\gamma), \quad (16)$$

$$\dot{s}^\lambda = s^\nu \ddot{x}_\nu \dot{x}^\lambda, \quad (17)$$

where f^μ is derived in Appendix B and its explicit form is given in equation (B6). In other words, the phase space in this description consists of $(x^\mu, \dot{x}^\nu, \ddot{x}^\kappa, s^\lambda)$. When we compare these variables with that of the KS condition, we see that even though we are not evolving any auxiliary w^λ , we do, however, store additional data in the acceleration vector \ddot{x}^λ . A recent discussion of this degeneracy of the MP condition was given by Costa *et al.* [47].

2.3. The TD condition

The Tulczyjew-Dixon supplementary spin condition [48, 49] $S^{\mu\nu}P_\nu = 0$ leads to the MPD equations of motion where we substitute \dot{x}^μ throughout by [50, 51]

$$\dot{x}^\mu = \frac{m}{\mathcal{M}^2} \left(P^\mu + \frac{2S^{\mu\nu}R_{\nu\gamma\kappa\lambda}P^\gamma S^{\kappa\lambda}}{4\mathcal{M}^2 + R_{\chi\eta\omega\xi}S^{\chi\eta}S^{\omega\xi}} \right), \quad (18)$$

where \mathcal{M} is an integral of motion, $\dot{\mathcal{M}} = 0$. The other mass m is not an integral of motion, and can be easily expressed as a function of $P^\mu, S^{\kappa\lambda}, R_{\alpha\beta\gamma\delta}$ from $\dot{x}^\mu \dot{x}_\mu = -1$ as

$$m = \frac{\mathcal{A}\mathcal{M}^2}{\sqrt{\mathcal{A}^2\mathcal{M}^2 - \mathcal{B}S^2}}, \quad (19)$$

$$\mathcal{A} = 4\mathcal{M}^2 + R_{\alpha\beta\gamma\delta}S^{\alpha\beta}S^{\gamma\delta}, \quad (20)$$

$$\mathcal{B} = 4h^{\kappa\eta}R_{\kappa\iota\lambda\mu}P^\iota S^{\lambda\mu}R_{\eta\nu\omega\pi}P^\nu S^{\omega\pi}. \quad (21)$$

The phase space is then parametrized by $(x^\mu, P^\nu, S^{\kappa\lambda})$.

Once again, there is the possibility to transform to a spin vector which yields [cf. 52]

$$\dot{P}^\mu = \frac{1}{\mathcal{M}} \star R_{\nu\kappa\lambda}^\mu \dot{x}^\nu s^\kappa P^\lambda, \quad (22)$$

$$\dot{s}^\mu = \frac{1}{\mathcal{M}^3} \star R_{\gamma\nu\kappa\lambda} S^{\gamma\lambda} \dot{x}^\nu s^\kappa P^\lambda P^\mu, \quad (23)$$

where we use equation (18) to eliminate \dot{x}^ν . This set of equations is non-linear and complicated, but the phase space is now composed only of (x^μ, P^ν, s^κ) , which is probably the most economic set of variables possible.

2.4. The CP and NW conditions

The Corinaldesi-Papapetrou (CP) [53] and Newton-Wigner (NW) [54, 55] condition employ an external time-like vector field $\xi^\mu(x^\nu)$ in the supplementary condition

$$S^{\mu\nu} \left(\xi_\nu + \alpha \frac{P_\nu}{\mathcal{M}} \right) = 0, \quad (24)$$

where $\alpha = 0$ corresponds to the CP and $\alpha = 1$ to the NW condition. The convenience of these supplementary conditions lies in the fact that one can recast the evolution for the spin tensor in terms of a tetrad basis $S^{AB} = e_\mu^A e_\nu^B S^{\mu\nu}$ and by choosing for instance $e_\mu^0 = \xi_\mu$ we can eliminate 3 of the six independent spin-tensor components $S^{0I}, I = 1, 2, 3$ as

$$S^{0I} = -\frac{\alpha}{\mathcal{M} + \alpha P_0} P_J S^{JI}, \quad J = 1, 2, 3. \quad (25)$$

The equations of motion for the spin tensor are obtained with the help of (6) as

$$\dot{S}^{\mu\nu} = 2S^{\kappa[\mu} \dot{x}^{\nu]} \frac{(\mathcal{M}\xi_{\kappa;\lambda} - \alpha R_{\hat{\kappa}\lambda\gamma\delta} S^{\gamma\delta} / 2) \dot{x}^\lambda}{(\mathcal{M}\xi_\chi + \alpha P_\chi) \dot{x}^\chi}, \quad (26)$$

where the notation $\hat{\kappa}$ in the curvature tensor signifies the part orthogonal to P^ν .

The momentum-velocity relation then attains the following implicit form

$$m\dot{x}^\mu = P^\mu - (S^{\kappa\mu} + S^{\kappa\omega}\dot{x}_\omega\dot{x}^\mu) \frac{(\mathcal{M}\xi_{\kappa;\lambda} - \alpha R_{\hat{\kappa}\lambda\gamma\delta} S^{\gamma\delta}/2)\dot{x}^\lambda}{(\mathcal{M}\xi_\chi + \alpha P_\chi)\dot{x}^\chi}. \quad (27)$$

This relation is not exactly reversible into a $\dot{x}^\mu(P_\nu)$ or $P_\nu(\dot{x}^\mu)$ formula in the general case and one thus cannot always use the CP/NW condition to give a set of evolution equations in strictly closed form.

Nevertheless, it is possible to iterate the momentum-velocity relation by starting from $\dot{x}^\mu = P^\mu/m + \mathcal{O}(S)$ to obtain results of higher and higher precision with respect to powers of S . The first iteration yields

$$m\dot{x}^\mu = P^\mu - \left(S^{\kappa\mu} + \frac{1}{m^2} S^{\kappa\omega} P_\omega P^\mu \right) \frac{\xi_{\kappa;\lambda} P^\lambda}{(m\xi_\chi + \alpha P_\chi) P^\chi} + \mathcal{O}(S^2). \quad (28)$$

Formulas such as the one above inserted into the MPD equations along with the assumption that (25) is exactly true at all times lead to closed-form evolution equations with the phase space (x^μ, P_ν, S^{IJ}) . By counting the variables, we see that the NW and CP conditions lead to systems with the same ‘‘minimal’’ number of degrees of freedom as the TD+MPD equations. One other reason the NW condition received heightened attention in the recent years is the fact that it can be formulated as a Hamiltonian system with the canonical $SO(3)$ commutation relations for the spin vector [34, 56, 57].

3. HAMILTONIANS FOR SPINNING PARTICLES

In this section we construct Hamiltonian formulations of the MPD equations supplemented by various choices of spin conditions. Besides being of fundamental interest, these are often advantageous for certain applications. For instance, in forthcoming sections we study a numerical integration of the MPD equations using efficient symplectic integrators on phase space. EOB waveform models use Hamiltonians to encode the conservative binary dynamics since they can naturally be mapped between the case of two bodies and a reduced mass in a fixed (effective) background.

3.1. The Poisson brackets

Before we are able to discuss Hamiltonians, we need to set up the stage in the form of a phase space endowed with a Poisson bracket. Consider the set of non-zero Poisson brackets for

the phase-space coordinates $x^\mu, P_\nu, S^{\gamma\kappa}$

$$\{x^\mu, P_\nu\} = \delta_\nu^\mu, \quad (29a)$$

$$\{P_\mu, P_\nu\} = -\frac{1}{2} R_{\mu\nu\kappa\lambda} S^{\kappa\lambda}, \quad (29b)$$

$$\{S^{\mu\nu}, P_\kappa\} = -\Gamma_{\lambda\kappa}^\mu S^{\lambda\nu} - \Gamma_{\lambda\kappa}^\nu S^{\mu\lambda}, \quad (29c)$$

$$\{S^{\mu\nu}, S^{\kappa\lambda}\} = g^{\mu\kappa} S^{\nu\lambda} - g^{\mu\lambda} S^{\nu\kappa} + g^{\nu\lambda} S^{\mu\kappa} - g^{\nu\kappa} S^{\mu\lambda}. \quad (29d)$$

This set of brackets arises in many models for spinning-particle dynamics [34, 58–63] and we provide our own motivation from field theory in Appendix C. Furthermore, it is easy to prove that the Poisson brackets follow from the generic effective action used in Refs. [21, 57, 64] (see Appendix E).

The Poisson brackets (29) can be partially canonicalized by choosing an orthonormal tetrad $e_\mu^A, e_\mu^A e^{\mu B} = \eta^{AB}$ (= Minkowski metric), and adopting a set of variables [59–61]

$$S^{AB} = S^{\mu\nu} e_\mu^A e_\nu^B, \quad (30)$$

$$p_\mu = P_\mu - \frac{1}{2} e_{\nu A;\mu} e_B^\nu S^{AB} = P_\mu - \frac{1}{2} \Gamma_{\nu\kappa\mu} S^{\nu\kappa}. \quad (31)$$

Under this change of variables the only non-zero brackets read

$$\{x^\mu, p_\nu\} = \delta_\nu^\mu, \quad (32a)$$

$$\{S^{AB}, S^{CD}\} = \eta^{AC} S^{BD} - \eta^{AD} S^{BC} + \eta^{BD} S^{AC} - \eta^{BC} S^{AD}. \quad (32b)$$

In this coordinate basis it is clear that S^{AB} and its commutation relations are a representation of the generators of the Lorentz group. Additionally, we see that $2S^2 = S^{AB} S_{AB} = S^{\mu\nu} S_{\mu\nu}$ and $2(S^*)^2 \equiv S^{A\hat{B}} S^{CD} \epsilon_{ABCD} = S^{\mu\nu} S^{\kappa\lambda} \epsilon_{\mu\nu\kappa\lambda}$ are Casimir elements of this algebra. That is, the spin magnitudes S, S^* commute with all the phase-space coordinates and will always be integrals of motion independent of the Hamiltonian.

However, if we compare with the MPD equations (5), we see that

$$\frac{d}{d\tau}(S^2) = S_{\mu\nu} \dot{S}^{\mu\nu} = 2S_{\mu\nu} p^\mu \dot{x}^\nu. \quad (33)$$

In other words, for conditions such as NW/CP that have $\dot{S} \neq 0$, the herein presented bracket will either not have any corresponding Hamiltonian, or the Hamiltonian dynamics will describe the NW/CP+MPD system indirectly through some deformed (non-MPD) set of variables.

3.2. Hamilton’s equations of motion

We are now in a position to study the equations of motion for a generic Hamiltonian $H(x^\mu, P_\nu, S^{\kappa\lambda})$ with the Poisson

brackets (29). We obtain

$$\frac{dx^\mu}{d\lambda} = \frac{\partial H}{\partial P_\mu}, \quad (34a)$$

$$\frac{dP_\nu}{d\lambda} + \frac{\partial H}{\partial x^\nu} - \frac{\partial H}{\partial S^{\mu\kappa}} (\Gamma^\mu_{\nu\gamma} S^{\gamma\kappa} + \Gamma^\kappa_{\nu\gamma} S^{\mu\gamma}) = -\frac{1}{2} R_{\nu\omega\lambda\chi} \frac{\partial H}{\partial P_\omega} S^{\lambda\chi}, \quad (34b)$$

$$\frac{dS^{\gamma\kappa}}{d\lambda} + \Gamma^\gamma_{\nu\lambda} \frac{\partial H}{\partial P_\nu} S^{\lambda\kappa} + \Gamma^\kappa_{\nu\lambda} \frac{\partial H}{\partial P_\nu} S^{\gamma\lambda} = \frac{\partial H}{\partial S^{\mu\nu}} (g^{\gamma\mu} S^{\kappa\nu} - g^{\gamma\nu} S^{\kappa\mu} + g^{\kappa\nu} S^{\gamma\mu} - g^{\kappa\mu} S^{\gamma\nu}), \quad (34c)$$

where λ is some parameter along the trajectory. These equations cannot be expected to make any sense on the full phase space, but only on the part where some supplementary condition $S^{\mu\nu} V_\nu = 0$ holds.

By comparison with equations (5), the equations (34) will be the MPD equations when the following equalities are fulfilled

$$\begin{aligned} \frac{\partial H}{\partial S^{\mu\nu}} (g^{\gamma\mu} S^{\kappa\nu} + \text{perm.}) &\cong P^\kappa \frac{\partial H}{\partial P_\gamma} - P^\gamma \frac{\partial H}{\partial P_\kappa}, \quad (35) \\ \frac{\partial H}{\partial x^\nu} - \frac{\partial H}{\partial S^{\mu\kappa}} (\Gamma^\mu_{\nu\gamma} S^{\gamma\kappa} + \Gamma^\kappa_{\nu\gamma} S^{\mu\gamma}) &\cong -\Gamma^\alpha_{\beta\nu} \frac{\partial H}{\partial P_\beta} P_\alpha, \quad (36) \end{aligned}$$

where \cong means that the equalities need to hold only on a certain ‘‘on-shell’’ part of the phase space where conditions such as $S^{\mu\nu} V_\nu = 0$ hold. The fact that the equalities are \cong makes them impractical to solve directly and we resort to heuristic approaches.

3.3. Hamiltonian for KS condition

Khriplovich [61] postulated the following Hamiltonian for semi-classical spinning particles which is to be used along the Poisson brackets (29) (see also d’Ambrosi *et al.* [63])

$$H_{\text{KS}} = \frac{1}{2m} g^{\mu\nu} P_\mu P_\nu \cong -\frac{m}{2}. \quad (37)$$

However, at the time of the publication of this Hamiltonian it was not clear what is the relation of the generated set of equations with the MPD equations. Nevertheless, we can now compare the generated equations of motion (34) with those corresponding to the relatively recently discovered KS supplementary spin condition (13) to see that the two sets of equation agree.

In other words, the Hamiltonian (37) generates the MPD equations under the KS spin condition. The only requirement that needs to be fulfilled by the initial condition apart from four-velocity normalization is for $S^{\mu\nu}$ to have some vanishing time-like direction w^ν , $S^{\mu\nu} w_\nu = 0$.

3.4. Hamiltonian for TD condition

Our initial heuristic is to simply reproduce the momentum-velocity relation under the TD condition and see whether this

is sufficient to determine the correct Hamiltonian. We take the velocity-momentum relation (18) and combine it with (34a) to obtain

$$\frac{\partial H}{\partial P_\nu} \cong \frac{m}{M^2} \left(P^\nu + \frac{2S^{\nu\mu} R_{\mu\gamma\kappa\lambda} P^\gamma S^{\kappa\lambda}}{4M^2 + R_{\chi\eta\omega\xi} S^{\chi\eta} S^{\omega\xi}} \right). \quad (38)$$

Now let us assume that the equations of motion hold under the on-shell conditions $\mathcal{M} = \sqrt{-P^\alpha P_\alpha}$, $S^{\mu\nu} P_\nu = 0$ where \mathcal{M} is now some chosen constant independent of phase-space coordinates. Then the following holds

$$\frac{\partial}{\partial P_\omega} [(g^{\mu\nu} P_\mu P_\nu + \mathcal{M}^2) F] \cong 2F P^\omega, \quad (39)$$

$$\frac{\partial}{\partial P_\omega} (G_\mu S^{\mu\nu} P_\nu) \cong G_\mu S^{\mu\omega}, \quad (40)$$

where F, G_μ are arbitrary functions of the phase-space coordinates $x^\kappa, P_\lambda, S^{\gamma\delta}$. By choosing appropriate F, G_μ , we are able to reproduce all the terms on the right hand side of (38) and thus obtain the Hamiltonian

$$\begin{aligned} H_{\text{TD}} = \frac{m}{2M^2} \left[\left(g^{\mu\nu} - \frac{4S^{\nu\gamma} R^\mu_{\gamma\kappa\lambda} S^{\kappa\lambda}}{4M^2 + R_{\chi\eta\omega\xi} S^{\chi\eta} S^{\omega\xi}} \right) P_\mu P_\nu \right. \\ \left. + \mathcal{M}^2 \right] \cong 0, \quad (41) \end{aligned}$$

where we substitute the expression (19) for m . A straightforward computation of Hamilton’s equations of motion then shows that they agree with the MPD equations of motion under the TD supplementary condition.

An interesting fact discussed in Appendix D is that the Hamiltonian (for a different time parametrization, $\lambda \neq \tau$) can be obtained by applying $S^{\mu\nu} P_\nu = 0$ as a Hamiltonian constraint of the Khriplovich Hamiltonian (37). However, this procedure does not seem to work for any other supplementary condition.

3.5. The MP Hamiltonian

Similarly to the TD condition, we are now looking for a Hamiltonian that generates the MP momentum-velocity relation (15)

$$\frac{\partial H}{\partial P_\mu} \cong \frac{1}{m} P^\nu \left(\delta^\mu_\nu - \frac{1}{S^2} S^{\mu\kappa} S_{\nu\kappa} \right). \quad (42)$$

We can compose it from the single on-shell condition $P_\mu P_\nu (g^{\mu\nu} - S^{\mu\kappa} S^\nu_{\kappa}/S^2) = -m^2$ similarly to the previous section (m is now a fixed number independent of the phase-space variables) to obtain

$$H_{\text{MP}} = \frac{1}{2m} \left(g^{\mu\nu} - \frac{1}{S^2} S^{\mu\kappa} S^\nu_{\kappa} \right) P_\mu P_\nu \cong -\frac{m}{2}. \quad (43)$$

Once again, the computation of the equations of motion shows that they are identical to the MPD equations under the MP condition.

3.6. Linear NW and CP Hamiltonian?

Let us try to reproduce the linearized NW/CP momentum-velocity relation (28)

$$\frac{\partial H}{\partial P_\mu} = \frac{1}{m} P^\mu - \left(S^{\kappa\mu} + \frac{1}{m^2} S^{\kappa\omega} P_\omega P^\kappa \right) \frac{\xi_{\kappa;\lambda} P^\lambda}{(m\xi_\chi + \alpha P_\chi) P^\chi}. \quad (44)$$

We use the on-shell condition $P^\mu P_\mu = -m^2 + \mathcal{O}(S^2)$ and $S^{\kappa\mu}(\alpha P_\mu/m + \xi_\mu) = 0$ to build the unique Hamiltonian that reproduces the relation above

$$H_{\text{NW/CP}} = \frac{1}{2m} g^{\mu\nu} P_\mu P_\nu - \frac{1}{\alpha} \frac{\xi_{\kappa;\lambda} P^\lambda}{(m\xi_\chi + \alpha P_\chi) P^\chi} S^{\kappa\mu} \left(\alpha \frac{P_\mu}{m} + \xi_\mu \right). \quad (45)$$

However, the computation of Hamilton's equations related to this Hamiltonian show that they are *not* a set of MPD equations. It is thus probably possible to cast the NW/CP+MPD system into Hamiltonian form only through a more sophisticated set of variables such as in Refs. [34, 56, 57, 65].

3.7. Coordinate-time parametrization

All of the above-stated Hamiltonians (37), (41), and (43) generate motion parametrized by proper time τ . It is possible to generalize them to any time parametrization λ with $d\lambda/d\tau$ an arbitrary function of any variables by exploiting the fact that the Hamiltonians have a constant value for any trajectory. We can then get the new λ -Hamiltonians as

$$H_\lambda = \left(\frac{d\lambda}{d\tau} \right)^{-1} (H_\tau - H_0). \quad (46)$$

The constant H_0 is $-m/2$ for the KS and MP Hamiltonians (37) and (43), and 0 for the TD Hamiltonian (41). These Hamiltonians evolve the full set of variables $x^\mu, P_\nu, S^{\gamma\kappa}$.

However, it is also possible to use the component of "non-covariant" momentum p_t from Eq. (31) expressed as a function of the other variables to generate the equations of motion parametrized by coordinate time t . To show this in the simplest possible way, we pass to the coordinates p_μ, S^{AB} defined in equations (30) and (31). We compute

$$\frac{dp_i}{dt} = -\frac{\partial H}{\partial x^i} \left(\frac{\partial H}{\partial p_t} \right)^{-1} = -\frac{\partial(-p_t)}{\partial x^i} \Big|_{H=\text{const.}}, \quad (47)$$

$$\frac{dx^i}{dt} = \frac{\partial H}{\partial p_i} \left(\frac{\partial H}{\partial p_t} \right)^{-1} = \frac{\partial(-p_t)}{\partial p_i} \Big|_{H=\text{const.}}, \quad (48)$$

$$\begin{aligned} \frac{dS^{AB}}{dt} &= \{S^{AB}, S^{CD}\} \frac{\partial H}{\partial S^{CD}} \left(\frac{\partial H}{\partial p_t} \right)^{-1} \\ &= \{S^{AB}, S^{CD}\} \frac{\partial(-p_t)}{\partial S^{CD}} \Big|_{H=\text{const.}}, \end{aligned} \quad (49)$$

where we have used the implicit function theorem. In other words, for any phase-space function $F(x^i, P_i, S^{AB})$

$$\frac{dF}{dt} = \{F, -p_t \Big|_{H=\text{const.}}\}. \quad (50)$$

We now list the respective Hamiltonians $H_t = -p_t \Big|_{H=\text{const.}}$ for the KS, TD, and MP spin conditions, given here in terms of the phase-space coordinates $P_\mu, S^{\kappa\lambda}$

$$H_{t\text{KS}} = -P_i \tilde{\omega}^i + \sqrt{\alpha^2 m^2 + \gamma^{ij} P_i P_j} + \frac{1}{2} \Gamma_{\nu\kappa t} S^{\nu\kappa}, \quad (51)$$

$$\omega^i \equiv -\frac{g^{ti}}{g^{tt}}, \quad \alpha \equiv \frac{1}{\sqrt{-g^{tt}}}, \quad \gamma^{ij} = -\frac{g^{ij}}{g^{tt}} + \omega^i \omega^j, \quad (52)$$

$$H_{t\text{TD}} = -P_i \tilde{\omega}^i + \sqrt{\tilde{\alpha}^2 \mathcal{M}^2 + \tilde{\gamma}^{ij} P_i P_j} + \frac{1}{2} \Gamma_{\nu\kappa t} S^{\nu\kappa}, \quad (53)$$

$$\tilde{g}^{\mu\nu} \equiv g^{\mu\nu} + \frac{4S^{\gamma(\nu} R^{\mu)}_{\gamma\kappa\lambda} S^{\kappa\lambda}}{4\mathcal{M}^2 + R_{\chi\eta\omega\xi} S^{\chi\eta} S^{\omega\xi}}, \quad (54)$$

$$\tilde{\omega}^i \equiv -\frac{\tilde{g}^{ti}}{\tilde{g}^{tt}}, \quad \tilde{\alpha} \equiv \frac{1}{\sqrt{-\tilde{g}^{tt}}}, \quad \tilde{\gamma}^{ij} = -\frac{\tilde{g}^{ij}}{\tilde{g}^{tt}} + \tilde{\omega}^i \tilde{\omega}^j, \quad (55)$$

$$H_{t\text{MP}} = -P_i \bar{\omega}^i + \sqrt{\bar{\alpha}^2 m^2 + \bar{\gamma}^{ij} P_i P_j} + \frac{1}{2} \Gamma_{\nu\kappa t} S^{\nu\kappa}, \quad (56)$$

$$\bar{g}^{\mu\nu} \equiv g^{\mu\nu} - \frac{1}{S^2} S^{\mu\kappa} S^{\nu\kappa}, \quad (57)$$

$$\bar{\omega}^i \equiv -\frac{\bar{g}^{ti}}{\bar{g}^{tt}}, \quad \bar{\alpha} \equiv \frac{1}{\sqrt{-\bar{g}^{tt}}}, \quad \bar{\gamma}^{ij} = -\frac{\bar{g}^{ij}}{\bar{g}^{tt}} + \bar{\omega}^i \bar{\omega}^j, \quad (58)$$

where we have chosen roots of p_t corresponding to particles traveling forward in time.

Now the reduced set of variables, to be evolved by the spatial part of the Poisson brackets (29) and the Hamiltonians above, are $x^i, P_j, S^{\mu\kappa}$. Alternatively, one can rewrite the Hamiltonians using the variables x^i, p_j, S^{AB} and use the spatial part of the brackets (32).

4. CANONICAL COORDINATES AND NUMERICAL INTEGRATION

In this section, we elaborate on the structure of the phase space. Being a geometric space (symplectic manifold), constraints can be viewed as defining a surface/submanifold. The projection of the Poisson bracket into the constraint surface leads to the so-called Dirac bracket [66, 67]. Furthermore, canonical coordinates can be adopted (at least locally), which we construct explicitly. This is crucial for the symplectic integration studied in the next section.

4.1. Importance of canonical coordinates and Dirac brackets

Let us assume that we have a set of constraints $\Phi^a = 0$ and the constraint algebra $C^{ab} = \{\Phi^a, \Phi^b\}$ with C^{ab} a non-degenerate matrix with an inverse C_{ab}^{-1} . Then it is possible to define a new constrained Poisson bracket [66, 67]

$$\{A, B\}' = \{A, B\} - \{A, \Phi^a\} C_{ab}^{-1} \{\Phi^b, B\}. \quad (59)$$

The bracket $\{, \}'$ is often called the Dirac or Dirac-Poisson bracket. If we have a Hamiltonian that fulfills $\{\Phi^a, H\} \cong 0$, then the equations of motion generated by $\{, \}'$ and H are the same as with $\{, \}$ and H . The bracket-constraining procedure was originally devised for the purposes of canonical quantization. Nonetheless, it is also useful for classical Hamiltonian dynamics.

When we want to study a classical Hamiltonian system at high accuracy over a large number of periods (such as would be the case of EMRIs), it is highly advantageous to use symplectic integration [see e.g. 68]. Most symplectic integrators require that the equations are formulated in terms of pairs of canonical coordinates, i.e. a collection of phase-space coordinates χ^i, π_i , with i some labelling index, such that $\{\chi^i, \pi_j\} = \delta_j^i$ (however, there do exist symplectic integrators for special classes of systems that require no such coordinates [69, 70]).

The usefulness of the constrained bracket $\{, \}'$ in this context can be twofold. First, it may be easier to find canonical coordinates for $\{, \}'$ rather than $\{, \}$. Second, the constraints $\Phi^a = 0$ are only integrals of motion with respect to the dynamical system evolved by the unconstrained bracket $\{, \}$, and they cannot be forced to be zero during integration, otherwise the advantageous properties of the symplectic algorithm are broken. On the other hand, in the case of the bracket $\{, \}'$, the constraints Φ^a commute with any phase-space variable. In return, they are effectively promoted to a “phase-space identity” and can be used to reduce the number of variables in a numerical integrator symplectic with respect to $\{, \}'$.

For example, Barausse *et al.* [34] applied the NW supplementary condition as a constraint to the bracket (32) (along with brackets and constraints for auxiliary variables) to obtain, at least at linear order in spin, a simplified bracket for the reduced number of variables p_μ, x^ν, S^{IJ} (see Subsection 2.4). This system was then easy to cover by approximate canonical coordinates and thus to study by symplectic integration [71].

As for the possibility to reduce the variables in the case of other supplementary conditions, the TD condition $S^{\mu\nu} P_\nu = 0$ applied as a constraint leads to a very complicated Dirac bracket that mixes the spin and momentum degrees of freedom. As a result, it is very difficult to find the canonical coordinate basis for the TD-constrained bracket.

On the other hand, as discussed in Subsections 2.1 and 2.2, the KS and MP condition in fact do not allow to reduce the number of evolved variables to the same extent as the TD and NW/CP conditions. A closer inspection shows that the KS and MP conditions cannot even be formulated as a constraint on the phase space p_μ, x^ν, S^{AB} , and the Poisson bracket will thus always be (32). Hence, for the purposes of the TD, KS, and MP conditions we have decided to find the canonical coordinates covering the full phase-space p_μ, x^ν, S^{AB} for the unconstrained bracket (32).

4.2. Canonical coordinates on S^{AB}

The p_μ, x^ν sector of the phase-space coordinates is already canonical, so we are looking for canonical coordinates covering the spin tensor S^{AB} . To find the canonical coordinates,

we mimic the procedure of Tessmer *et al.* [72] by expressing S^{AB} as a simple constant tensor $S^{\hat{A}\hat{B}}$ in some “body-fixed frame” plus a Lorentz transformation $\Lambda^A_{\hat{A}}$ into the “background frame” e^A_μ . The parameters of the transformation, when chosen appropriately, then turn out to be canonically conjugate pairs of coordinates.

The details of the procedure are given in Appendix E, we only summarize here the resulting coordinates

$$A = S^{12} - \sqrt{(S^{12})^2 + (S^{23})^2 + (S^{31})^2}, \quad (60a)$$

$$B = \sqrt{(S^{12})^2 + (S^{23})^2 + (S^{31})^2} - S, \quad (60b)$$

$$\phi = -\arctan\left(\frac{S^{23}}{S^{31}}\right), \quad (60c)$$

$$\psi = -\arctan\left(\frac{S^{23}}{S^{31}}\right) - \arccos\left(S^{03}\sqrt{C}\right), \quad (60d)$$

$$C = \frac{(S^{12})^2 + (S^{23})^2 + (S^{31})^2}{[(S^{13})^2 + (S^{32})^2][(S^{01})^2 + (S^{02})^2 + (S^{03})^2]}. \quad (60e)$$

Even though the construction in Appendix E provides the path to the derivation of these coordinates, one may simply verify their Poisson brackets by direct computation. The brackets then are $\{\phi, A\} = \{\psi, B\} = 1$ and 0 otherwise.

The backwards transformations from the canonical coordinates to the spin tensor read

$$S^{01} = \mathcal{D} [A \cos(2\phi - \psi) + (A + 2B + 2S) \cos \psi], \quad (61a)$$

$$S^{02} = \mathcal{D} [A \sin(2\phi - \psi) + (A + 2B + 2S) \sin \psi], \quad (61b)$$

$$S^{03} = 2\mathcal{D}\mathcal{E} \cos(\phi - \psi), \quad (61c)$$

$$S^{12} = A + B + S, \quad (61d)$$

$$S^{23} = -\mathcal{E} \sin \phi, \quad (61e)$$

$$S^{31} = \mathcal{E} \cos \phi, \quad (61f)$$

$$\mathcal{D} = -\frac{\sqrt{B(B+2S)}}{2(B+S)}, \quad (61g)$$

$$\mathcal{E} = \sqrt{-A(A+2B+2S)}. \quad (61h)$$

The coordinates cover the space of general antisymmetric tensors with a degenerate time-like direction and a closer consideration reveals a number of similarities with hyperspherical coordinates in \mathbb{R}^4 .

The coordinates have singularities at $B = 0$ and $A = 0, -2(B + S)$ which have the character similar to those of the singularities at $r = 0$ and $\cos(\vartheta) = 1, -1$ in spherical coordinates in \mathbb{R}^3 . As a result, the physical coordinate ranges then are $B \in (0, \infty)$ and $A \in (-2(B + S), 0)$. The coordinates ϕ, ψ are simple angular coordinates similar to the azimuthal angle φ in spherical coordinates in \mathbb{R}^3 , and they both run in the $[0, 2\pi)$ interval. Some more details about the coordinate singularities are given in Appendix E.

One last remark is that the coordinates ϕ, ψ are dimensionless and have finite limits as $S \rightarrow 0$, whereas A, B have the dimension of the spin and should generally go to zero when $S \rightarrow 0$. However, if we keep $a \equiv A/S, b \equiv B/S$ finite, then the evolution of the coordinates a, b, ϕ, ψ can be used to track

the evolution of a “test spin”, i.e. an intrinsic spin of the particle that is transported along the trajectory while not exerting any back-reaction on the orbit itself.

There is a special case when A, B can remain finite while $S \rightarrow 0$, and that corresponds to the body-fixed frame being infinitely boosted with respect to the background frame and the vanishing direction of the spin tensor becoming light-like. This particular limit may be useful for the description of massless particles with spin but we consider it to be physically meaningless for the current context of massive bodies.

5. SPECIAL PLANAR MOTION

We now want to study a simple restricted problem that would allow us to demonstrate the properties of the canonical coordinates. We do so by considering a motion in the equatorial plane of the Schwarzschild space-time under the KS condition. Then we require that both the four-velocity and the spin tensor are initially vanishing in the ϑ direction, $S^{\mu\vartheta} = 0, \dot{\vartheta} = 0$. We then easily compute that

$$\frac{d^2\vartheta}{d\tau^2} = 0, \quad (62)$$

$$\frac{dS^{\mu\vartheta}}{d\tau} = 0. \quad (63)$$

In other words, the conditions $S^{\mu\vartheta} = 0, \dot{\vartheta} = 0$ will be satisfied throughout the motion.

A similar system restricted to the equatorial plane can be formulated by requiring $P_{\vartheta} = S^{\mu\vartheta} = 0$ also for the MP and TD conditions, and, furthermore, the background could be generalized to the Kerr space-time. However, we choose here to study the special planar problem only in the KS incarnation and in the Schwarzschild space-time because of its simplicity.

It should also be noted that this system is *more general* than the motion of a particle with the spin vector aligned normal to the equatorial plane; such motion can be acquired from the system described below by setting $B = 0$. However, for $B \neq 0$ the motion is different from the aligned-spin case. The spin vector undergoes nutations and exerts non-uniform torques on the orbit that, nonetheless, never push the worldline out of the equatorial plane.

5.1. The Hamiltonian

For our computations, we choose the coordinate-aligned tetrad in the usual Schwarzschild coordinates t, φ, r, ϑ : $e_{\mu}^0 = \sqrt{-g_{tt}}\delta_{\mu}^t, e_{\mu}^1 = \sqrt{g_{\varphi\varphi}}\delta_{\mu}^{\varphi}, e_{\mu}^2 = \sqrt{g_{rr}}\delta_{\mu}^r, e_{\mu}^3 = \sqrt{g_{\vartheta\vartheta}}\delta_{\mu}^{\vartheta}$. The choice of the tetrad and even the order of the legs are important for the final form of the Hamiltonian and the physical interpretation of the quantities appearing in it. However, the choice of the tetrad never matters for the real physical evolution of the KS, TD, or MP conditions (unlike in the case of the NW/CP condition where the choice $\sim \xi^{\mu} \sim e_{\mu}^{\nu}$ is crucial [73]).

The condition $S^{\vartheta\mu} = 0$ then translates into either $A = 0$ or $A = -2(B + S)$ for $S^{12} > 0$ and $S^{12} < 0$ respectively. Here we choose $S^{12} > 0$, and ϕ thus becomes a redundant coordinate (see more details in Appendix E). In a typical right-hand-oriented interpretation and for an orbit with positive $\dot{\varphi}$, this corresponds to a spin vector counter-aligned to the orbital angular-momentum vector.

When the dust settles, the Hamiltonian (37) expressed in canonical coordinates in the case of the special planar motion reads

$$H_{\text{SP}} = \frac{1}{2m} \left[\frac{-1}{1 - 2M/r} \left(p_t - \frac{M\sqrt{B(B+2S)}\sin\psi}{r^2} \right)^2 + \left(1 - \frac{2M}{r} \right) p_r^2 + \frac{1}{r^2} \left(p_{\varphi} - \sqrt{1 - \frac{2M}{r}}(B+S) \right)^2 \right]. \quad (64)$$

The system has two obvious integrals of motion p_{φ}, p_t , since the coordinates t, φ are cyclic. However, it should be noted that the orbital angular momentum and energy will generally vary during the evolution since they relate to the phase-space coordinates as

$$u_t = \frac{1}{m} \left(p_t - \frac{M\sqrt{B(B+2S)}\sin\psi}{r^2} \right), \quad (65)$$

$$u_{\varphi} = \frac{1}{m} \left(p_{\varphi} - \frac{r^{5/2}(B+S)}{\sqrt{r-2M}} \right). \quad (66)$$

5.2. Poincaré surfaces of section

We have constructed the problem so that only two degrees of freedom become dynamically important, r, p_r , and ψ, B . Since the trajectory is also constrained by four-velocity normalization, all the phase-space trajectories of a given p_{φ}, p_t are then confined to a 3-dimensional hypersurface. We make a natural Poincaré surface of section through this hypersurface by sampling this set of trajectories and recording the phase-space variables every time ψ finishes a 2π cycle. Thanks to this construction, we obtain well-defined 2D Poincaré surface of section, whereas in the general case the surface of section becomes higher-dimensional and new methods need to be employed for visualization [see 74].

We have integrated the trajectories using the 6-th order Gauss collocation scheme with a fixed-point iteration of the collocation points [see, e.g., 68]. Additionally, we exploited the parametrization invariance of the trajectory by using a time parameter λ such that

$$\frac{d\lambda}{d\tau} = \frac{r_0^2}{r(r-2M)} \frac{S}{\sqrt{B(B+2S)+\epsilon}}, \quad (67)$$

where ϵ, r_0 are constants we set to $10^{-4}, 10M$ respectively. This effective time-stepping does not spoil the symplecticity of the integrator because the respective equations of motion can be generated by a Hamiltonian of the form (46).

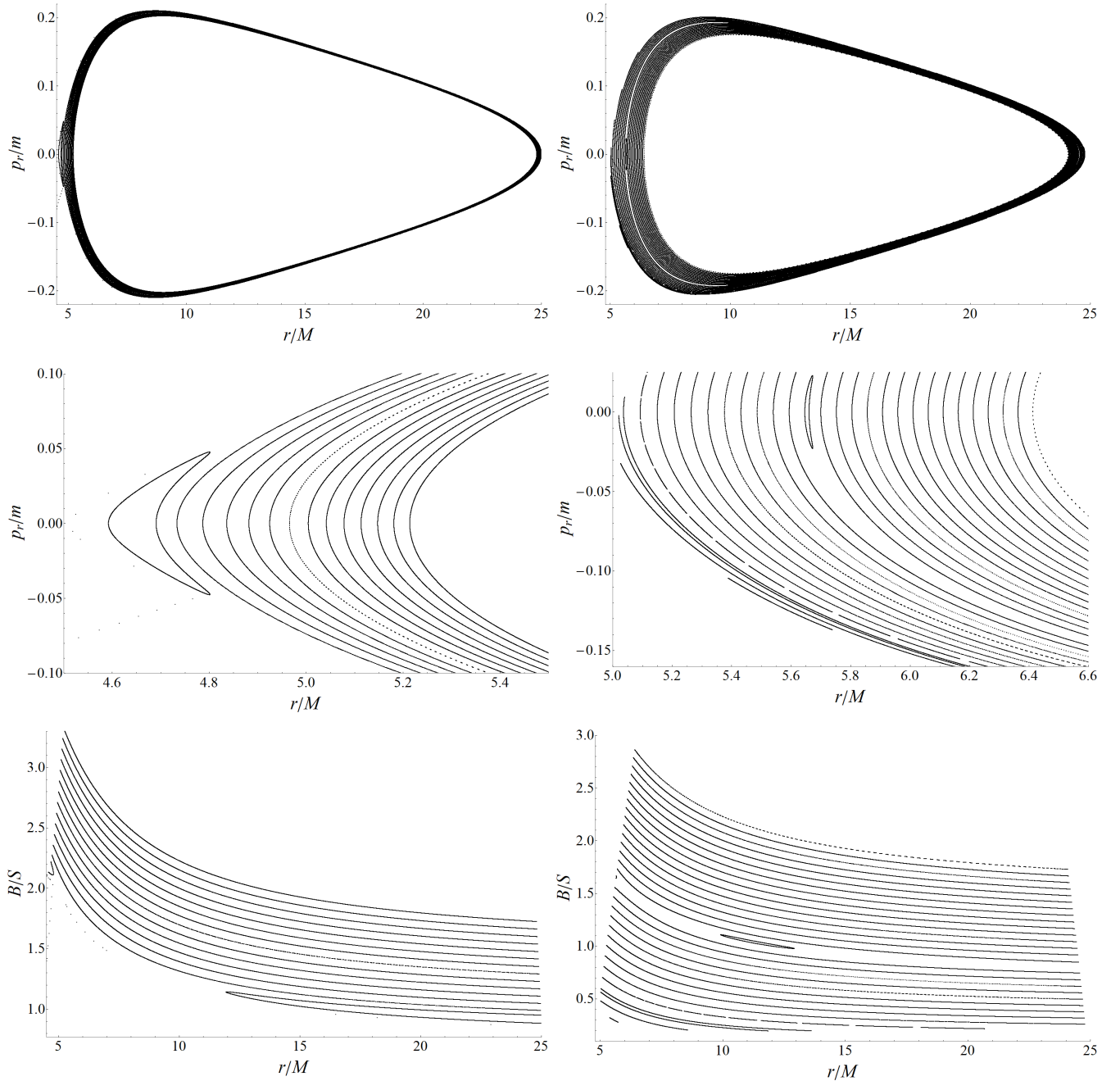


FIG. 1. Poincaré surfaces of section for the special planar problem at $p_t/m = -0.97, p_\varphi/m = 3.7M$ created by snapshots after every cycle in the spin-angle ψ . The left column corresponds to $S/m = 0.05M$ and the right column to $S/m = 0.1M$. The outer parts of the nested sections correspond to small B/S whereas the inner parts to growing B/S . The left column features a smaller number of orbits because the “outer” orbits are plunging into the black hole.

With these measures in place and by using a standard single-thread computation in C++, we were able to integrate through 10^4 spin cycles within minutes at a relative error less than 10^{-12} in the four-velocity normalization. Of course, such efficiency and long-term accuracy would hardly be possible without the canonical coordinates and geometrical integration. This is an important point of the present section.

In general, the dimensionless parameter $S/(Mm)$ can

be understood as a perturbation strength non-linearly coupling two exactly integrable systems, the geodesic motion in Schwarzschild space-time, and the parallel transport of the “test spin” on top of that geodesic. As such, the dependence of the phase portrait of the special planar problem on the particle spin should have the same characteristics as any weakly non-integrable system [e.g. 75]: The originally smooth phase-space foliation by regular oscillations of the trajectories should

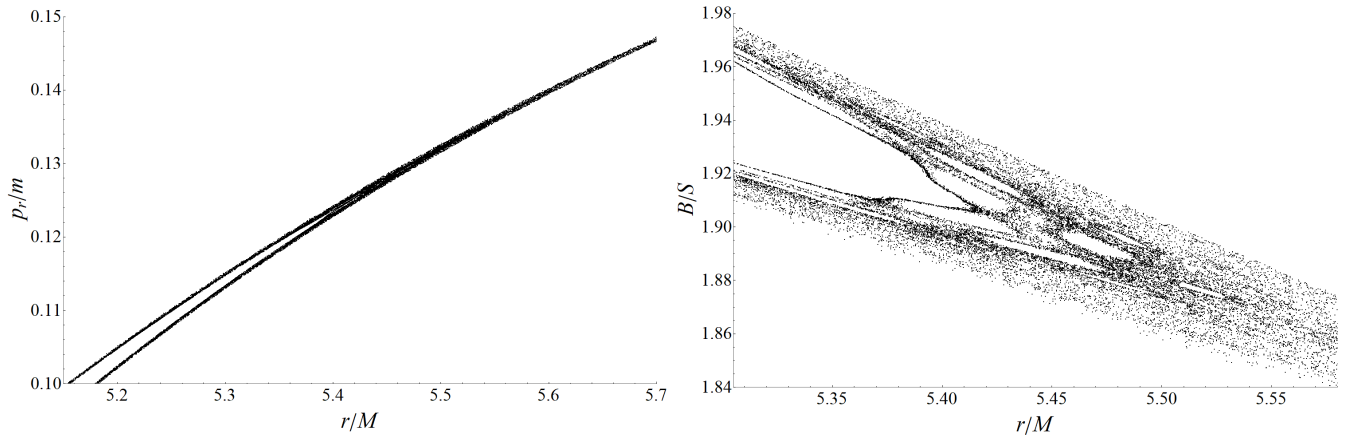


FIG. 2. A detailed Poincaré surface of section of a single chaotic trajectory at $p_t/m = -0.97$, $p_\varphi/m = 3.7M$, $S/m = 0.05M$ (compare with left column of Fig. 1). The trajectory was integrated over $\sim 10^5$ spin cycles ($\sim 10^4$ orbital cycles) so that we would observe its release from the sticky fractal layer around the resonance into the general separatrix chaos.

now feature occasional “breaks” in the form of resonances and thin chaotic layers.

In order to demonstrate the presence of such structures, we probed values of p_t, p_φ so that phase-space trajectories in the studied congruence are near unstable circular orbits in the original geodesic flow. This is because the neighboring phase space also contains the “homoclinic” infinite whirl-zoom orbits that are well known to act as “seeds of chaos” in perturbed black hole space-times [see, e.g., 76–79]. However, as can be seen from equations (65) and (66), the variations of S also have the unfortunate effect of shifting the meaning of p_t, p_φ , and this easily pushes us into the phase-space regions of orbits plunging into the black hole.

As already discussed in the Introduction, we should be already imposing self-force effects along with the spin-force even for the smallest values of $S/(mM)$ in a self-consistent physical model. Thus, it does not make sense to study the influence of the spin beyond perturbation-like values and we choose to study only $S/(mM) \leq 0.1$.

Furthermore, the ratio B/S is equal to $\gamma - 1$, where γ is the usual gamma factor of the Lorentz boost from the body-fixed frame to the background frame (see Appendix E). The unconstrained nature of the KS condition allows this γ to be arbitrary, but we believe that if it becomes too large, the world-line becomes shifted outside of the interior of the real physical body, and the system of equations instead obtains the character of some sort of perturbed geodesic-deviation equation. Hence, we only allow $B/S \lesssim 5$ in our initial conditions.

We show two Poincaré surfaces of section in the relevant ranges in Fig. 1. In these sections, we are able to find resonances corresponding to ratios as low as 1 : 1 or 1 : 2 in the spin-orbital frequencies. Additionally, small chaotic layers can be found near the saddle points of the resonant chains (see Fig. 2).

As we go to smaller values of $S/(mM) \lesssim 0.01$, the resonances become extremely thin, and most of the chaotic structure is disqualified based on the criterion $B/S \lesssim 5$. If we ignore the B/S criterion and go to $B/S \gtrsim 10$, chaos can be

found up to $S/(mM) \sim 10^{-3}$.

5.3. Comparison with previous results

Let us briefly compare these results with the study of Lukes-Gerakopoulos *et al.* [74], who studied the chaotization of general orbits of spinning particles in Kerr space-time while using the NW-condition Hamiltonian of Barausse *et al.* [34]. The motion of non-planar orbits with general spin orientations leads to richer dynamics, as an additional degree of freedom enters the interactions. Consequently, Lukes-Gerakopoulos *et al.* found chaotic motion in the phase space until $S/(mM) = 10^{-3}$.

At face value, it might not be clear whether our findings are in tension or in agreement with those of Lukes-Gerakopoulos *et al.* [74]. As discussed in Subsection 2.4, the NW condition constrains one more degree of freedom than the KS condition. Consequently, an analogous special planar motion $P^\vartheta = \dot{x}^\vartheta = S^{\mu\vartheta} = 0$ would in fact have only a single active degree of freedom under the NW condition and would thus be integrable at any value of spin. Additionally, even the non-planar motion under the NW Hamiltonian of Barausse *et al.* [34] is integrable to linear order in S in Schwarzschild space-time, at least under the right choice of ξ^μ [73].

In this sense, we are adding a result to this chain of research by showing that the KS+MPD system is not integrable in Schwarzschild space-time even in the planar case. Hence, one should be cautious in issuing general statements about the (non)-integrability and chaos in MPD equations near black holes, because such statements seem to be dependent on the context and approximations made.

6. CONCLUSIONS AND OUTLOOKS

In this paper we have built the Hamiltonian formalism for spinning particles under all commonly used “comoving” sup-

plementary conditions, that is, conditions that utilize only the local dynamics of the body and no background vector field. The full set of canonical coordinates that we provide is the minimal set of variables needed to evolve the Mathisson-Pirani and Kyrian-Semerák conditions. Hence, our formalism allows to integrate the respective equations at peak efficiency. However, the canonical coordinates contain a redundant degree of freedom for the case of the Tulczyjew-Dixon condition. Nevertheless, a pair of extra variables to be evolved in a numerical routine is a small price to pay for the long-term quality of the evolution such as the one seen in Section 5.

Of course, it would be interesting to see whether a minimal set of canonical coordinates can be found for the Tulczyjew-Dixon condition. In principle, this can be achieved by constraining the Poisson bracket similarly to Barausse *et al.* [34], and by finding the canonical basis thereof. However, the constraint procedure introduces non-zero commutation relations between momenta, space-time coordinates, and spin degrees of freedom. Consequently, the canonical coordinates would in fact be an intricate transformation of all p_μ, x^μ, S^{AB} . We plan to investigate this possibility in future work.

Another less obvious application of the canonical coordinates is the fact that now we are able to formulate a Hamilton-Jacobi equation by making the action \mathcal{S} also a function of the spin angles ψ, ϕ with the gradients defining the conjugate momenta $\mathcal{S}_{,\phi} = A, \mathcal{S}_{,\psi} = B$. We are currently preparing a

manuscript presenting solutions to the Hamilton-Jacobi equation in black hole space-times.

Similarly, we believe that the herein presented formalism can be very useful to the various averaging and two-timescale approaches to EMRIs [18, 80–82] since we can easily construct action-angle coordinates in the spin sector and thus provide an elegant treatment of the non-dissipative (“fast”) part of the dynamics of the binary. Furthermore, the simplicity of the Hamiltonian under the Kyrian-Semerák condition makes it an attractive alternative to the Hamiltonian of Barausse *et al.* [34] in EOB models [83].

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Appendix A: The generalized KS conditions

The only condition that we need to be fulfilled for $\dot{S}^{\kappa\lambda} = 0$ to hold is that $\dot{S}^{\mu\nu}w_\nu = 0$ for some time-like w^ν . From equation (6) projected into w^ν we then get

$$w^\nu \dot{x}_\nu \dot{S}^{\kappa\lambda} = 0. \quad (\text{A1})$$

Because the product of any two time-like vectors is non-zero, we then get simply $\dot{S}^{\kappa\lambda} = 0$. The supplementary condition can thus be of the form $S^{\mu\nu}w_\nu = m^\mu$ with

$$S^{\mu\nu}\dot{w}_\nu = \dot{m}^\mu, \quad (\text{A2})$$

because then we will have $\dot{S}^{\mu\nu}w_\nu = 0$. In the case when $m^\mu = 0$, we get that \dot{w}_ν must lay in the degenerate directions of the spin tensor, $\dot{w}_\nu = \alpha w_\nu + \beta s_\nu$ with α, β arbitrary functions of any variables [84]. However, we may generally set $m^\mu \neq 0$ and then the only condition on the evolution is Eq. (A2). One particular option is $\dot{w}^\mu = \dot{m}^\mu = 0$.

Nevertheless, it should be noted that only the initial choices of w^μ, m^ν matter. This can be seen from the fact that if the equations of motion are expressed in terms of $S^{\mu\nu}$, we need no reference to \dot{w}^μ, \dot{m}^ν as long as equation (A2) is satisfied.

In summary, once we allow for $m^\mu \neq 0$, the initial conditions for $S^{\mu\nu}$ are completely unconstrained. The study of d'Ambrosi *et al.* [85] can be understood as conducted exactly in the $m \neq 0$ generalized KS condition.

One last note is that the vector m^μ represents a mass dipole in the frame w^μ , and by setting its dynamics to fulfill different evolution equations than in Eq. (A2), we can in fact obtain other supplementary conditions [86].

Appendix B: The expression for \ddot{x}^μ under MP condition

Take the equations (5) and (7) to express

$$(m\dot{x}^\mu + \dot{x}_\gamma \dot{S}^{\gamma\mu})' = -\frac{1}{2}R_{\nu\kappa\lambda}^{\mu} \dot{x}^\nu S^{\kappa\lambda}. \quad (\text{B1})$$

Now use $S^{\mu\nu}\dot{x}_\nu = 0$ along with its time-derivatives and the fact that $\dot{x}_\gamma \ddot{x}^\gamma = 0, \dot{x}_\gamma \dot{P}^\gamma = 0$ to obtain [46]

$$m\ddot{x}^\mu - \ddot{x}_\gamma S^{\gamma\mu} = -\frac{1}{2}R_{\nu\kappa\lambda}^{\mu} \dot{x}^\nu S^{\kappa\lambda}. \quad (\text{B2})$$

We now contract the expression above with $S_{\nu\mu}/S^2$ and partially re-express the result using the spin vector s^λ to obtain

$$\begin{aligned} \ddot{x}^\kappa \left(\delta_\kappa^\nu + \dot{x}_\kappa \dot{x}^\nu - \frac{s_\kappa s^\nu}{S^2} \right) &= \frac{m}{S^2} \ddot{x}^\mu S_{\mu}^\nu \\ &+ \frac{1}{2S^2} R_{\mu\lambda\kappa\gamma} \dot{x}^\lambda S^{\nu\mu} S^{\kappa\gamma}. \end{aligned} \quad (\text{B3})$$

That is, we now have the expression for the jerk \ddot{x}^ν on the subspace orthogonal to $s^\lambda, \dot{x}^\kappa$. The projection of the jerk into velocity can be computed from the second derivative of four-velocity normalization as $\ddot{x}^\mu \dot{x}_\mu = -\dot{x}^\mu \ddot{x}_\mu$. For the projection of the jerk into the spin vector, we use the Fermi-transport property $\dot{s}^\mu = -\dot{s}^\nu \dot{x}_\nu \dot{x}^\mu$ to express $\dot{s}^\nu \dot{x}_\nu = 0$. This allows us rewrite the projection as

$$s^\mu \ddot{x}_\mu = \frac{D}{d\tau}(s^\mu \dot{x}_\mu). \quad (\text{B4})$$

Now let us project Eq. (B2) into s^μ to obtain

$$s^\mu \ddot{x}_\mu = -\frac{1}{2m} R_{\mu\nu\kappa\lambda} s^\mu \dot{x}^\nu S^{\kappa\lambda}. \quad (\text{B5})$$

We now see that the time-derivative of $\ddot{x}^\mu s_\mu$ can be completely expressed by known functions of $x^\mu, \dot{x}^\nu, \ddot{x}^\kappa, s^\lambda$.

From that, it is now easy to compose the complete prescription for the jerk only in terms of the variables $\dot{x}^\mu, \ddot{x}^\lambda, s^\gamma$ as

$$\ddot{x}^\nu = \frac{1}{S^2} (m\ddot{x}_\mu - \star R_{\mu\lambda\kappa\gamma} \dot{x}^\lambda s^\kappa \dot{x}^\gamma) \epsilon^{\nu\mu\sigma\tau} \dot{x}_\sigma s_\tau + \ddot{x}^\kappa \dot{x}_\kappa \dot{x}^\nu + \frac{1}{mS^2} \left(\star R_{\mu\lambda\kappa\gamma; \sigma} s^\mu \dot{x}^\lambda s^\kappa \dot{x}^\gamma \dot{x}^\sigma + 2\star R_{\mu\lambda\kappa\gamma} s^\mu s^\kappa \dot{x}^\lambda \ddot{x}^\gamma \right) s^\nu. \quad (\text{B6})$$

Appendix C: Field-theoretic motivation for Poisson brackets

We assume a fixed 3+1 split of space-time which consists of a family of non-intersecting spatial hypersurfaces Σ_t (we will suppress the t in the following) with coordinates x^i and induced metric d_{ij} , volume element $d\Sigma = \sqrt{d} d^3x$. This means that our time parametrization is fixed and what we expect to find is not strictly the parametrization-invariant Poisson bracket (29), but rather a constrained bracket with new terms in the temporal sector [see 56, 67, for more details].

We can then take a Lagrangian density $\mathcal{L} = \tilde{\mathcal{L}}\sqrt{-g}$ ($\tilde{\mathcal{L}}$ is the Lagrangian scalar) and obtain a Hamiltonian density using the usual Legendre transformation

$$\pi_a = \frac{\partial \mathcal{L}}{\partial (\partial_t \phi^a)}, \rightarrow \partial_t \phi_a = f(\pi_b, \phi^b, \dots), \quad (\text{C1})$$

$$\mathcal{H}(\pi_b, \phi^b, \dots) = \frac{\partial \mathcal{L}}{\partial (\partial_t \phi^a)} \partial_t \phi^a - \mathcal{L}, \quad (\text{C2})$$

where ϕ^a stands for a generic collection of fields. Note that π_a is a density on Σ (*not* in the whole space-time). In the fol-

lowing we will always assume that all the fields and momenta vanish smoothly at the boundary of Σ (spatial infinity).

This system now has the non-zero local Poisson brackets (meaningful only when evaluated for fields at the same t)

$$\{\phi^a(x^i, t), \pi_b(y^j, t)\} = \delta_b^a \delta^{(3)}(x^i - y^j), \quad (\text{C3})$$

where we can generate brackets for gradients by commuting the gradient with the bracket. It can be shown that this generates a Poisson bracket for functionals

$$A(t)[\pi, \phi] = \int \mathcal{A}(\pi_a, \pi_{a,i}, \phi, \phi_{,i}^a, x^i, t) d^3x, \quad (\text{C4})$$

$$B(t)[\pi, \phi] = \int \mathcal{B}(\pi_a, \pi_{a,i}, \phi, \phi_{,i}^a, x^i, t) d^3x, \quad (\text{C5})$$

$$\{A(t), B(t)\} = \int \frac{\delta \mathcal{A}}{\delta \phi^a} \frac{\delta \mathcal{B}}{\delta \pi_a} - \frac{\delta \mathcal{B}}{\delta \phi^a} \frac{\delta \mathcal{A}}{\delta \pi_a} d^3x, \quad (\text{C6})$$

where \mathcal{A}, \mathcal{B} are densities on Σ and $\delta \mathcal{F} / \delta f$ is the variational derivative

$$\frac{\delta \mathcal{F}}{\delta f} = \frac{\partial \mathcal{F}}{\partial f} - \frac{\partial}{\partial x^i} \frac{\partial \mathcal{F}}{\partial (f_{,i})}, \quad (\text{C7})$$

where we have assumed that \mathcal{F} is dependent only on f and its first-order gradients (for higher order gradients we get a series of analogous terms of varying sign).

1. Total momentum

We define a particular momentum quantity Π_μ that will play an analogous role as the covariant momentum P_μ

$$\Pi_\mu(t) \equiv - \int_\Sigma T_\mu^\nu n_\nu d\Sigma, \quad (\text{C8})$$

where n_ν is the unit normal to Σ .

For this expression, we choose the canonical stress-energy tensor generated by diffeomorphism invariance rather than the Hilbert stress-energy tensor

$$T_\mu^\nu = \frac{\partial \tilde{\mathcal{L}}}{\partial (\phi_{,\nu}^a)} \phi_{,\mu}^a - \delta_\mu^\nu \tilde{\mathcal{L}}. \quad (\text{C9})$$

The momentum can then be rewritten as

$$\Pi_\mu(t) = - \int \pi_a \phi_{,\mu}^a - \delta_\mu^t \mathcal{L} d^3x. \quad (\text{C10})$$

Namely, we have

$$\Pi_t = - \int \mathcal{H} + \gamma_{tb}^a \pi_a \phi^b d^3x, \quad (\text{C11})$$

where $\gamma_{\mu b}^a$ are some connection coefficients for the covariant derivative of the fields ϕ^a , $\phi_{,\mu}^a = \phi_{,\mu}^a + \gamma_{\mu b}^a \phi^b$.

We require that $(\phi^a \pi_a)_{,\mu} = (\phi^a \pi_a)_{;\mu}$ and the validity of the Leibniz rule, which leads us to the definition of the pseudo-covariant derivative of π_a as $\pi_{a;\mu} = \pi_{a,\mu} - \gamma_{\mu a}^b \pi_b$. This convention is at odds with the usual convention for the covariant

gradient of a density; its intuitive meaning is that $\pi_{a;\mu}$ is rather some kind of ‘‘total density variation’’ of π_a .

Since $\{\phi^a(x^i, t), \mathcal{H}(y^j, t)\} = \partial_t \phi(x^i, t) \delta^{(3)}(x^i - y^j)$ then we get

$$\{\phi^a(x^i, t), \Pi_t\} = -\phi_{,t}^a - \gamma_{tb}^a \phi^b = -\phi_{;t}^a(x^i, t). \quad (\text{C12})$$

For the spatial part we obtain similarly

$$\{\phi^a(x^j, t), \Pi_i\} = - \int \{\phi^a, \pi_b \phi_{;i}^b\} d^3x = -\phi_{;i}^a(x^j, t). \quad (\text{C13})$$

For the momenta we obtain analogously

$$\{\pi_a(x^i, t), \Pi_\mu\} = -\pi_{a,\mu} + \gamma_{\mu a}^b \pi_b = -\pi_{a;\mu}(x^i, t). \quad (\text{C14})$$

That is, at least for functions of fields and momenta which do not involve their gradients, $\{\cdot, \Pi_\mu\}$ is minus the covariant gradient operator.

2. Mutual momentum brackets

Let us compute the bracket $\{\Pi_\mu, \Pi_\nu\}$. We start with

$$\begin{aligned} \{\Pi_i, \Pi_t\} &= \iint \{\pi_c(\phi_{,i}^c + \gamma_{id}^c \phi^d), \mathcal{H} + \gamma_{tb}^a \pi_a \phi^b\} d^3x d^3y \\ &= -2 \int \pi_{c;[i} \phi_{;t]}^c d^3x. \end{aligned} \quad (\text{C15})$$

The spatial brackets then yield

$$\begin{aligned} \{\Pi_i, \Pi_j\} &= \iint \{\pi_c(\phi_{,i}^c + \gamma_{id}^c \phi^d), \pi_a(\phi_{,j}^a + \gamma_{jd}^a \phi^d)\} d^3x d^3y \\ &= -2 \int \pi_{c;[i} \phi_{;j]}^c d^3x. \end{aligned} \quad (\text{C16})$$

In summary $\{\Pi_\mu, \Pi_\nu\} = -2 \int \pi_{c;[\mu} \phi_{;\nu]}^c d^3x$. On the other hand, in the brackets (29) we have $\{P_\mu, P_\nu\} = -R_{\alpha\beta\mu\nu} S^{\alpha\beta} / 2$.

We try to simplify the brackets further, starting with $\{\Pi_i, \Pi_j\}$. To do that we reexpress

$$\pi_{c;i} \phi_{;j}^c = (\pi_c \phi_{;j}^c)_{,i} - \pi_c \phi_{|ji}^c, \quad (\text{C17})$$

$$\begin{aligned} \phi_{|ji}^c &\equiv \phi_{,ji}^c + \gamma_{ib}^c \phi_{,j}^b + \gamma_{jb}^c \phi_{,i}^b + \gamma_{jb,i}^c \phi^b + \gamma_{jb}^c \gamma_{ia}^b \phi^a \\ &= \phi_{;ji}^c - \Gamma_{ji}^k \phi_{,k}^c, \end{aligned} \quad (\text{C18})$$

Even though $\phi_{|ij}^c$ is missing a part to be fully covariant with respect to the background space-time, its antisymmetric part is in fact covariant and yields

$$\phi_{|ji}^c - \phi_{|ij}^c = R_{bj i}^c \phi^b. \quad (\text{C19})$$

We then assume that the field vanishes at the boundaries of Σ and obtain

$$\{\Pi_i, \Pi_j\} = \int \pi_{c;j} \phi_{;i}^c - \pi_{c;i} \phi_{;j}^c d^3x = - \int R_{bij}^a \pi_a \phi^b d^3x. \quad (\text{C20})$$

For the $\{\Pi_t, \Pi_i\}$ bracket we can use a similar trick but some of the gradients will be with respect to t and do not integrate out to boundary terms. As a result, we obtain

$$\{\Pi_i, \Pi_t\} = - \int R^a_{bit} \pi_a \phi^b d^3x + \int (\pi_c \phi^c_{;i}, t) d^3x. \quad (\text{C21})$$

In summary

$$\{\Pi_\mu, \Pi_\nu\} = - \int R^a_{b\mu\nu} \pi_a \phi^b d^3x + \delta_\mu^t \frac{d\Pi_\nu}{dt} - \delta_\nu^t \frac{d\Pi_\mu}{dt}. \quad (\text{C22})$$

This is an *exact* relation for an arbitrary collection of fields vanishing at infinity and an arbitrary 3+1 split. Note that for a single scalar field the first term vanishes and we probably cannot get anything resembling the Poisson brackets (29). In the next Section we briefly describe a formal expansion of this relation.

3. “Monopole” approximation

We now assume that the fields ϕ^a, π_b are non-vanishing only over a small volume as compared to the variability length of the curvature. Then we can expand the integral from the $\{\Pi_\mu, \Pi_\nu\}$ bracket as

$$\begin{aligned} \int R^a_{b\mu\nu} \pi_a \phi^b d^3x &= R^a_{b\mu\nu}(x^i_W, t) \int \pi_a \phi^b d^3x \\ &+ R^a_{b\mu\nu;k}(x^i_W, t) \int X^k \pi_a \phi^b d^3x \\ &+ \dots, \end{aligned} \quad (\text{C23})$$

where x^i_W is some referential point inside the volume where the fields are non-vanishing, and the vector field $X^k(x^i, x^i_W, t)$ can be constructed, e.g., as the gradient of Synge’s world function around x^i_W [87]. If we take only the first term of this expansion, we obtain

$$\begin{aligned} \{\Pi_\mu(t), \Pi_\nu(t)\} &= - \frac{1}{2} R^a_{b\mu\nu}(x^i_W, t) \mathcal{S}_a^b \\ &+ \delta_\mu^t \frac{d\Pi_\nu}{dt} - \delta_\nu^t \frac{d\Pi_\mu}{dt} + \dots, \end{aligned} \quad (\text{C24})$$

$$\mathcal{S}_a^b \equiv 2 \int \pi_a \phi^b d^3x, \quad (\text{C25})$$

where the spin tensor S^{AB} corresponds to the antisymmetric part of \mathcal{S}_a^b drawn into tetrad components.

4. $\{\mathcal{S}_a^b, \Pi_\mu\}$ bracket

Let us start with the spatial part,

$$\begin{aligned} \{\mathcal{S}_a^b, \Pi_i\} &= -2 \iint \{\pi_a \phi^b, \pi_c \phi^c_{;i}\} d^3x d^3y \\ &= -2 \int \pi_a \phi^b_{;i} + \pi_{a;i} \phi^b d^3x \\ &= -2 \int (\pi_a \phi^b)_{;i} + \gamma^b_{id} \pi_a \phi^d - \gamma^c_{ia} \pi_c \phi^b d^3x. \end{aligned} \quad (\text{C26})$$

The temporal part reads

$$\begin{aligned} \{\mathcal{S}_a^b, \Pi_t\} &= -2 \iint \{\pi_a \phi^b, \mathcal{H} + \gamma^c_{td} \pi_c \phi^d\} d^3x d^3y \\ &= -2 \int (\pi_a \phi^b)_{;t} + \gamma^b_{td} \pi_a \phi^d - \gamma^c_{ta} \pi_c \phi^b d^3x. \end{aligned} \quad (\text{C27})$$

The first term in the last line can be rewritten as $d\mathcal{S}_a^b/dt$.

Assuming again a leading-order expansion of the integrals we obtain

$$\{\mathcal{S}_a^b, \Pi_\mu\} = -\gamma^b_{\mu d} \mathcal{S}_a^d + \gamma^c_{\mu a} \mathcal{S}_c^b + \delta_\mu^t \frac{d\mathcal{S}_a^b}{dt} + \dots \quad (\text{C28})$$

This is in good correspondence to the respective Poisson bracket in (29).

5. $\{\mathcal{S}_a^b, \mathcal{S}_c^d\}$ bracket

$$\{\mathcal{S}_a^b, \mathcal{S}_c^d\} = \iint \{\pi_a \phi^b, \pi_c \phi^d\} d^3x d^3y = \delta_c^b \mathcal{S}_a^d - \delta_a^d \mathcal{S}_c^b. \quad (\text{C29})$$

The corresponding Poisson bracket in (29) contains additional terms that follow once we anti-symmetrize \mathcal{S}_a^b .

6. The world-line coordinate

The referential point for the “monopole” approximation defined above can be constructed as

$$x^i_W \equiv \frac{\int x^i f(\phi^a \pi_a) d^3x}{\int f(\phi^a \pi_a) d^3x} \quad (\text{C30})$$

With f an arbitrary differentiable, positive definite function of its argument. Then we can compute

$$\begin{aligned} \{x^j_W, \Pi_i\} &= - \frac{\int x^j f'(\phi^a \pi_a) (\phi^a \pi_a)_{;i} d^3x}{\int f(\phi^a \pi_a) d^3x} \\ &+ \frac{\int x^j f(\phi^a \pi_a) d^3x}{\int f(\phi^a \pi_a) d^3x} \frac{\int f'(\phi^a \pi_a) (\phi^a \pi_a)_{;i} d^3x}{\int f(\phi^a \pi_a) d^3x} \\ &= \frac{\int (x^j)_{;i} f(\phi^a \pi_a) d^3x}{\int f(\phi^a \pi_a) d^3x} = \delta^j_i. \end{aligned} \quad (\text{C31})$$

That is, this is exactly the canonically conjugate coordinate we are looking for.

The time coordinate t_W is just t . In principle, we can then write the commutation relation in a unified form that emphasizes the similarity with the other brackets and thus the terms coming from the time-parametrization constraint

$$\{x^\mu_W, \Pi_\nu\} = \delta^\mu_\nu - \delta_\nu^t \frac{dx^\mu_W}{dt}. \quad (\text{C32})$$

7. Discussion of field-theoretic motivation of Poisson bracket

The spin structure of the brackets comes from the internal field structure already in a monopole, rather than a pole-dipole approximation. However, for instance a perfect fluid can be described only by a set of scalar fields and would not generate these “spin dynamics”. Hence, the present “derivation” of the Poisson brackets is not a fundamental reasoning as to why such a set of brackets should apply to the motion of compact astrophysical objects. We thus understand the procedure given in this Appendix merely as one of the possible motivations for the Poisson brackets (29). The procedure above also provides an interesting field-theoretic background for the spinor and vector-based models of classical particles with spin [62, 88–91].

Attempts to derive brackets for higher-order multipoles break down as inelegant non-covariant terms start mixing into the expressions. We are convinced that for a generalization of the procedure above to higher multipoles, a more careful construction of the multipolar expansion must be given. Namely, definitions of “vector-like” quantities such as Π_μ are not covariant even with respect to coordinate changes on Σ and covariant definitions with similar properties must be found.

Appendix D: Constraining the Khrilovich Hamiltonian

1. Constraint theory

Let us first introduce some elements of Dirac-Bergmann constraint theory as presented, e.g., by Dirac [66], Hanson *et al.* [67].

Let $\Phi^a = 0$ be a set of constraints on phase space we want to impose on the system, with a some index labeling the constraints. Let us further assume that the matrix $C^{ab} \equiv \{\Phi^a, \Phi^b\}$ is non-degenerate and we can thus find an inverse matrix C_{ab}^{-1} . The goal is to find a Hamiltonian H' which fulfills $\{\Phi^a, H'\} = \dot{\Phi}^a \cong 0$, where \cong denotes an equality which is fulfilled under the condition that all the constraints $\Phi^a = 0$ hold. Such a Hamiltonian can be obtained from the original one as

$$H' = H - \{H, \Phi^a\} C_{ab}^{-1} \Phi^b. \quad (D1)$$

In our particular case we will be imposing the constraints of the form $S^{\mu\nu} V_\nu = 0$. By counting the components of the constraint, we might be tempted to state that there are a total of 4 constraints imposed on the system. However, two components of the constraint are satisfied trivially due to the identities $S^{\mu\nu} V_\nu V_\mu = 0$ and $S^{\mu\nu} V_\nu \star S_{\mu\kappa} V^\kappa = 0$. As a consequence, the matrix $C^{\mu\lambda} \equiv \{S^{\mu\nu} V_\nu, S^{\lambda\kappa} V_\kappa\}$ will be degenerate on subspaces corresponding to these trivial constraints. However, it can be easily seen that if we find any pseudo-inverse $C_{\mu\lambda}^\dagger$, then the following Hamiltonian will conserve the non-trivial parts of the constraint and thus also the whole set $S^{\mu\nu} V_\nu = 0$

$$H' = H - \{H, S^{\mu\nu} V_\nu\} C_{\mu\lambda}^\dagger S^{\lambda\kappa} V_\kappa. \quad (D2)$$

The last note to this procedure is that in the following we never constrain the Poisson algebra; in other words, the Pois-

son brackets are always those given in (29). More details about this topic are discussed in the main text in Section 4.

2. Obtaining the TD Hamiltonian

The first constraint that we apply to the Hamiltonian (37) is $S^{\mu\nu} P_\nu = 0$. The constraint algebra yields

$$\{S^{\mu\nu} P_\nu, S^{\kappa\lambda} P_\lambda\} \cong -\tilde{\mathcal{M}}^2 S^{\mu\kappa}, \quad (D3)$$

$$\tilde{\mathcal{M}}^2 \equiv -g^{\mu\nu} P_\mu P_\nu + \frac{1}{4} R_{\mu\nu\kappa\lambda} S^{\mu\nu} S^{\kappa\lambda}. \quad (D4)$$

The pseudo-inverse of $S^{\mu\kappa}$ on the constrained phase space is $-S_{\nu\mu}/S^2$ (cf. eq. (12)). The last bracket that needs to be evaluated is

$$\{H_{\text{KS}}, S^{\kappa\lambda} P_\lambda\} \cong \frac{1}{2m} R_{\mu\nu\gamma\chi} S^{\kappa\mu} P^\nu S^{\gamma\chi}. \quad (D5)$$

The constrained Hamiltonian then reads

$$\begin{aligned} H_{\text{TD}} &= \frac{1}{2\mu} g^{\mu\nu} P_\mu P_\nu + \{H_{\text{KS}}, S^{\kappa\lambda} P_\lambda\} \frac{1}{\tilde{\mathcal{M}}^2 S^2} S_{\mu\kappa} S^{\mu\nu} P_\nu \\ &= \frac{1}{2\mu} \left(g^{\mu\nu} + \frac{1}{\tilde{\mathcal{M}}^2} R_{\chi\xi\zeta}^\mu S^{\chi\nu} S^{\xi\zeta} \right) P_\mu P_\nu, \end{aligned} \quad (D6)$$

where we can apply \cong equalities for expressions multiplied by the constraint $S^{\mu\nu} P_\nu$ without changing the resulting equations of motion. We have also chosen to change the notation $m \rightarrow \mu$ because as we will see, the meaning of the parameter μ will be different from the definition (8). This Hamiltonian generates the equations of motion parametrized by some parameter λ which does not need to be equal to proper time τ . The equations of motion read

$$x'^\mu \cong \frac{1}{\mu} \left(g^{\mu\nu} + \frac{1}{2\tilde{\mathcal{M}}^2} R_{\chi\xi\zeta}^\nu S^{\chi\mu} S^{\xi\zeta} \right) P_\nu, \quad (D7)$$

$$P'^\mu \cong -\frac{1}{2} R_{\nu\kappa\lambda}^\mu x'^\nu S^{\kappa\lambda}, \quad (D8)$$

$$S'^{\mu\nu} \cong P^\mu x'^\nu - P^\nu x'^\mu, \quad (D9)$$

where we denote the derivatives $D/d\lambda$ by primes. By comparing the equations above with the MPD equations of motion under the TD supplementary condition (18) we see that the parameter λ fulfills

$$\frac{d\lambda}{d\tau} = \frac{\mu m}{\tilde{\mathcal{M}}^2}, \quad (D10)$$

where we substitute Eq. (19) for m . Another way to characterize the parametrization under the condition that $P^\alpha P_\alpha = -\mathcal{M}^2 = -\mu^2$ is that it holds that $P^\alpha x'_\alpha / \mathcal{M} = -1$. This is exactly the parametrization introduced by Dixon [49] and vouched for by Ehlers and Rudolph [50] (see also [92]). The Hamiltonian for world-lines parametrized by proper time is discussed in the main text in Subsection 3.4. One should compare the above-given constraint procedure with the analogous constraint procedure in the vector-variable model of Ramírez and Deriglazov [62].

3. Other attempts

We attempted to use the MP momentum-velocity relation (15) and thus to apply the constraint $S^{\mu\nu}(\delta_\nu^\kappa + S^{\kappa\lambda}S_{\lambda\nu}/S^2)P^\nu = 0$. The problem is, however, that once the spin tensor is degenerate, the identity $S^{\mu\nu}(\delta_\nu^\kappa + S^{\kappa\lambda}S_{\lambda\nu}/S^2) = 0$ holds automatically and has no time derivative under the Kriplovich Hamiltonian. In other words, the MP condition expressed in terms of momenta is satisfied by any degenerate spin tensor and it cannot be used in our constraint procedure.

The Corinaldesi-Papapetrou condition $S^{\mu\nu}\xi_\nu = 0$, where $\xi^\nu(x^\mu)$ is now some fixed vector field, can be applied as a constraint to yield the Hamiltonian

$$H = \frac{1}{2m}g^{\mu\nu}P_\mu P_\nu + \frac{1}{m\xi^2}\xi_{\nu;\gamma}P^\gamma S^{\nu\kappa}\xi_\kappa. \quad (\text{D11})$$

Yielding the equations of motion

$$x^{\prime\prime\mu} = -\frac{1}{2m}R^\mu_{\nu\kappa\lambda}x^{\prime\nu}S^{\kappa\lambda} - \frac{1}{\xi^2}\xi_{\nu;\gamma}x^{\prime\gamma}S^{\nu\kappa}\xi_{\kappa;\mu}, \quad (\text{D12})$$

$$S^{\prime\nu\kappa} = -\frac{1}{\xi^2}\xi_{\lambda;\gamma}x^{\prime\gamma}(S^{\lambda\nu}\xi^\kappa - S^{\kappa\lambda}\xi^\nu). \quad (\text{D13})$$

Nevertheless, this set of equations are not the MPD equations under the Corinaldesi-Papapetrou condition.

Appendix E: Construction of canonical coordinates

Consider the effective action for spinning bodies given in Steinhoff and Schaefer [64]:

$$S = \int p_\mu \dot{x}^\mu + \frac{1}{2}S_{AB}\Omega^{AB} - H d\tau, \quad (\text{E1})$$

where $\Omega^{AB} \equiv \Lambda^A_{\hat{A}} \frac{d\Lambda^{B\hat{A}}}{d\tau}$ and $\Lambda^A_{\hat{A}}$ are the components of the ‘‘body-fixed frame’’ with respect to the background tetrad e_μ^A . The body-fixed frame is defined by the property that the spin tensor is constant in it, $S^{\hat{A}\hat{B}} = \text{const.}$, and $\Lambda^A_{\hat{A}}$ thus in fact carry the dynamical state of the spin tensor along with gauge degrees of freedom. We further assume here, unlike in Refs. [21, 57, 64], that the Hamiltonian H is only a function of the gauge-independent p_μ, x^ν, S^{AB} . It is then easy to show that the equations of motion following from $\delta S = 0$, where $p_\mu, x^\nu, \Lambda^A_{\hat{A}}, S^{AB}$ are varied independently, imply

$$\frac{df}{d\tau} = \{f, H\}, \quad (\text{E2})$$

where f is any function of p_μ, x^ν, S^{AB} and the bracket is given as in Eq. (32). In this sense, our Hamiltonian-based approach can be understood, up to the discarding of the $\Lambda^A_{\hat{A}}$ variables, as equivalent to the action-based approach of Refs. [21, 57, 64].

We now realize that if the term $S_{AB}\Omega^{AB}/2$ can be transformed into the form $\sum_i \rho_i \dot{\chi}^i$ with ρ_i, χ^i some dynamical

variables, then ρ_i, χ^i are the desired pairs of canonically conjugate coordinates on the phase space. To do so, we mimic the approach presented in Tessmer *et al.* [72] and re-express

$$\frac{1}{2}S_{AB}\Omega^{AB} = \frac{1}{2}S_{\hat{A}\hat{B}}\Lambda^A_{\hat{A}}\Lambda^B_{\hat{B}}\Omega^{AB} = \frac{1}{2}S_{\hat{A}\hat{B}}\Lambda^A_{\hat{A}}\frac{d\Lambda^{B\hat{A}}}{d\tau}. \quad (\text{E3})$$

In other words, we are now looking at the dynamics of the spin tensor purely from the perspective of a Lorentz transformation $\Lambda^A_{\hat{A}}$ from the body-fixed frame into the referential tetrad.

We now choose the spin tensor in the body-fixed frame to have one degenerate time-like direction and one non-degenerate space-like direction; conventionally $S_{\hat{1}\hat{2}} = -S_{\hat{2}\hat{1}} = S$ and other components zero. Note that this assumes that the spin tensor will eventually fulfill a supplementary spin conditions of the form $S^{\mu\nu}V_\nu = 0$; non-degenerate spin tensors will thus not be possible to express in terms of the coordinates that we give in the following paragraphs.

To enable an intuitive discussion, let us further identify the legs $\Lambda^A_{\hat{1}}, \Lambda^B_{\hat{2}}, \Lambda^C_{\hat{3}}$ with the x, y, z -axes in Cartesian coordinates, and the $\Lambda^D_{\hat{0}}$ with the time axis. Then, by finding the dual of the spatial part of the spin tensor, we see that it is a vector of magnitude S pointing purely in the z -direction.

The spin tensor is invariant with respect to rotations around the z -axis, and with respect to boosts in the z direction. Out of the total 6 parameters of a general Lorentz transform $\Lambda^A_{\hat{A}}$, 2 will be gauge degrees of freedom of the body-fixed tetrad. In order to not mix the gauge degrees of freedom and the true dynamical degrees of freedom, we parametrize the general Lorentz transform as

$$\Lambda = R(\alpha, \vec{n}_z)B(v_z, \vec{n}_z)B(u, \vec{n}_\psi)R(-\theta, \vec{n}_\phi), \quad (\text{E4})$$

where $R(\zeta, \vec{n})$ stands for a rotation by angle ζ around \vec{n} , and $B(v, \vec{n})$ a boost in the \vec{n} direction. The numbers $\alpha, v_z, u, \psi, \theta, \phi$ are then generally time-dependent parameters of the transformation, and the vectors $\vec{n}_\psi, \vec{n}_\phi$ are given as

$$\vec{n}_\psi = (-\sin \psi, \cos \psi, 0), \quad (\text{E5})$$

$$\vec{n}_\phi = (-\sin \phi, \cos \phi, 0). \quad (\text{E6})$$

When the dust settles, this transformation yields

$$\begin{aligned} \frac{1}{2}S_{AB}\Omega^{AB} &= S\Lambda^{\hat{1}}_A \frac{d\Lambda^{A\hat{2}}}{d\tau} \\ &= -S\dot{\alpha} + S\frac{\cos \theta - 1}{\sqrt{1-u^2}}\dot{\phi} + S\left(\frac{1}{\sqrt{1-u^2}} - 1\right)\dot{\psi}. \end{aligned} \quad (\text{E7})$$

The $-S\dot{\alpha}$ term is a total time derivative and so it will not contribute to the equations of motion. From the other terms we see that we have two canonical momenta A and B conjugate to ϕ and ψ respectively defined through the parameters of the Lorentz transformation as

$$A = S\frac{\cos \theta - 1}{\sqrt{1-u^2}}, \quad (\text{E8})$$

$$B = S\left(\frac{1}{\sqrt{1-u^2}} - 1\right). \quad (\text{E9})$$

Expressions for these coordinates in terms of the components of the spin tensor are given in the main text in equation (60). The expressions for the spin tensor components in terms of A, B, ϕ, ψ are then given in equation (61).

1. Coordinate singularities and the special-planar Hamiltonian

Imagine a particle moving along $x = 0$ and $y = 0$ in Cartesian coordinates in Euclidean space, and make the usual transform to spherical coordinates r, ϑ, φ . In principle, the coordinate $\varphi = \arctan(x/y)$ is not defined, and we are at $\vartheta = 0$ or $\vartheta = \pi$ depending on the sign of z . By a limiting procedure $x \rightarrow 0, y \rightarrow 0$, we are able to obtain any value between 0 and 2π for φ at the pole.

However, it is clear to us from the point of view of the more fundamental Cartesian coordinates that nothing is wrong, as the value of φ is of no consequence for them at $\vartheta = 0$. Similarly, $\dot{\varphi}$ is not defined at the pole, and by taking the azimuthal angular momentum along with ϑ to zero, we obtain any value for $\dot{\varphi}$ between $-\infty$ and $+\infty$; again, this is of no physical consequence and evolving φ is redundant.

The singularity at the pole of spatial spherical coordinates is similar to the singularity of the canonical coordinates for the spin tensor at $S^{A3} = 0$. By inspecting the transformation laws (60) we see that the coordinate $\phi = -\arctan(S^{23}/S^{31})$ is undefined and we are either at $A = 0$ or $A = -2(B + S)$

depending on the sign of S^{12} .

In the case $A = 0$ ($S^{12} > 0$), we see from the parametrization of the spin tensor (61) that the value of ϕ will in fact be of no consequence to the spin tensor. These conclusions can then be easily applied to an evolution that fulfills $S^{A3} = \text{const.} = 0$ to reduce the number of variables we need to evolve.

In the case $A = -2(B + S)$ ($S^{12} < 0$) the situations is somewhat more complicated. If we have an evolution that keeps $S^{A3} = \text{const.} = 0$, we will also have $\dot{S}^{A3} = 0$. This, however, leads only to $\dot{A} = -2\dot{B}$, and it is in fact the combination $2\phi - \psi$ that uniquely parametrizes the spin tensor. For practical purposes, it then useful to define new canonical coordinates $D \equiv A/2 - B, E \equiv A/2 + B, \delta \equiv 2\phi - \psi, \epsilon \equiv 2\phi + \psi$ so that D, δ and E, ϵ are conjugate respectively. The equation $\dot{S}^{A3} = 0$ with $S^{12} < 0$ leads to $\dot{E} = 0$ and the redundancy of the coordinate ϵ .

For the special planar problem in Sec. 5, we chose $S^{12} > 0$ for simplicity. A trick that can be eventually used to avoid the redefinitions of coordinates is simply to permute the definition of the tetrad elements $1 \leftrightarrow 2$, which will lead to a change of the physical meaning of the sign of S^{12} .

Another singularity is at $S^{A0} = 0$ which unambiguously leads to $B = 0$ and ψ undefined. Once again, we see in (61) that the value of ψ is inconsequential in that case. An interesting fact is that if we have an evolution such that $S^{A0} = \text{const.} = 0$, then the coordinates A, ϕ reduce just to the canonical coordinates for the $SO(3)$ Poisson algebra [e.g. 71].