A Novel Energy-conserving Scheme for Eight-dimensional Hamiltonian Problems

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Abstract

We design a novel, exact energy-conserving implicit nonsymplectic integration method for an eight-dimensional Hamiltonian system with four degrees of freedom. In our algorithm, each partial derivative of the Hamiltonian with respect to one of the phase-space variables is discretized by the average of eight Hamiltonian difference terms. Such a discretization form is a second-order approximation to the Hamiltonian gradient. It is shown numerically via simulations of a Fermi–Pasta–Ulam–β system and a post-Newtonian conservative system of compact binaries with one body spinning that the newly proposed method has extremely good energy-conserving performance, compared to the Runge–Kutta; an implicit midpoint symplectic method, and extended phase-space explicit symplectic-like integrators. The new method is advantageous over very long times and for large time steps compared to the state-of-the-art Runge–Kutta method in the accuracy of numerical solutions. Although such an energy-conserving integrator exhibits a higher computational cost than any one of the other three algorithms, the superior results justify its use for satisfying some specific purposes on the preservation of energies in numerical simulations with much longer times, e.g., obtaining a high enough accuracy of the semimajor axis in a Keplerian problem in the solar system or accurately grasping the frequency of a gravitational wave from a circular orbit in a post-Newtonian system of compact binaries. The new integrator will be potentially applied to model time-varying external electromagnetic fields or time-dependent spacetimes.

Unified Astronomy Thesaurus concepts: Black hole physics (159); Computational methods (165); Computational astronomy (293); Chaos (222); Compact binary stars (283)

1. Introduction

Numerical integration schemes are convenient to handle many complicated nonlinear dynamical problems, such as the motion of relativistic charged particles in external electromagnetic fields (Kopáček & Karas 2014) and general relativistic systems of compact binaries consisting of black holes and/or neutron stars (Thorne & Hartle 1985; Kidder 1995; Buonanno et al. 2006). Although explicit Runge–Kutta (RK) integrators can generally give very accurate solutions to these systems, they are nonsymplectic/non-geometric methods that do not conserve the invariants of motion and, therefore, cause a secular, unphysical increase in energy errors even if these systems are conservative. In this sense, such non-geometric methods are generally discarded. Instead, geometric integration methods (Hairer et al. 2006) are usually used.

Without doubt, symplectic integrators (Ruth 1983; Feng & Qin 1987; Forest & Ruth 1990; Wisdom & Holman 1991; Zhong et al. 2010) are a class of geometric integration methods. They not only preserve symplectic structures of Hamiltonian systems but also show no intrinsic unbounded accumulation of energy errors due to their long-term numerical stability. Symmetric methods (Quinlan & Tremaine 1990) are similar to the symplectic integrators and do not lead to a secular, unphysical energy drift. Extended phase-space methods (Pihajoki 2015; Liu et al. 2016; Li & Wu 2017; Luo et al. 2017) are also explicitly symplectic-like or are symmetric schemes. As a point to note, the so-called conservation of energies in these integrators does not mean that these algorithms strictly conserve the energy integrals without any truncation errors from a theoretical viewpoint, but that does mean that these algorithms show no secular drift in the energy errors from a numerical viewpoint.

Are there a class of energy-conserving integrators that can exactly conserve the energy integral of a conservative Hamiltonian from the theoretical viewpoint? Yes, there are. As a path to obtain them, the gradient of the Hamiltonian is discretized by use of Hamiltonian difference terms so that the Hamiltonian can be exactly conserved numerically step by step. This conservation of the Hamiltonian of the system is said to be energy conservation. First-order discrete Hamiltonian gradient schemes were constructed by Chorin et al. (1978) and Feng (1985). The construction of such first-order Hamiltonian-conserving methods is simple, but those of second-order Hamiltonian-conserving schemes may be complicated. The second-order discretization of the Hamiltonian gradient depends on the dimension of the Hamiltonian. The second-order discrete gradient scheme for a four-dimensional Hamiltonian system with two degrees of freedom can be found in some references (Qin 1987; Itoh & Abe 1988; Wang et al. 2008; Feng & Qin 2009). The discretization of each partial derivative of the Hamiltonian with respect to one of the position and momentum variables is the average of four Hamiltonian difference terms. Recently, an extension to a six-dimensional Hamiltonian system with three degrees of freedom was given by Bacchini et al. (2018). Here, each component of the Hamiltonian gradient is replaced with the average of six Hamiltonian difference terms. The number of such average values adds up to six. This energy-conserving integration scheme was used to model time-like and null geodesics in

5 In the present paper, this presentation is only based on the general case in which the Hamiltonian represents some form of the energy of the system. If the Hamiltonian differs from the energy, then Hamiltonian-conserving does not mean energy-conserving.
general relativity (Bacchini et al. 2019). These exact energy-conserving algorithms are implicit and nonsymplectic.

It is worth pointing out that the exact conservation of energies is important during numerical studies of the long-term evolution of conservative systems in astrophysics. This requirement satisfies a physical need of conservative systems. In addition, it is based on a need of some specific purposes in numerical simulations with much longer times. For example, the Keplerian energy of a pure Keplerian two-body problem in the solar system closely depends on the orbital semimajor axis, mean motion, and mean anomaly (Murray & Dermott 1999). The conservation of the Keplerian energy in numerical simulations results in improving the accuracy of the semimajor axis, eliminating the Lyapunov instability of orbits, and suppressing the fast accumulation of numerical errors along the in-track direction. In particular, this leads to accurately grasping periodic motion (i.e., the orbital frequency of a circular, spherical or quasi-spherical orbit) in a system of two black holes (Kidder 1995) over long times—that is, accurately grasping the frequency of a gravitational wave emitted from the circular, spherical, or quasi-spherical orbit. This is because the frequency of the wave from the circular orbit doubles the frequency of the circular orbit.

Considering the importance of conserving energy in numerical integrations of long-term evolution of objects in astrophysics, we will generalize the work of Bacchini et al. (2018) and construct a new exact energy-conserving integration method for an eight-dimensional Hamiltonian with four degrees of freedom in the present paper. This scheme is also based on Hamiltonian differencing and replaces the Hamiltonian gradient with an approximation to the Hamiltonian gradient. This discrete average is still a second-order approximation to the Hamiltonian gradient. This is the main aim of this paper.

The paper is organized as follows. A new energy-conserving method is given in Section 2. Taking a Fermi–Pasta–Ulam (FPU)-β system (Skokos et al. 2008; Gerlach et al. 2012) as a tested model in Section 3, we check the numerical performance of the new method, compared to that of the RK method; the implicit midpoint rule (Feng 1986; Zhong et al. 2010; Mei et al. 2013) and extended phase-space methods (Pihajoki et al. 2015; Liu et al. 2016; Li & Wu 2017; Luo et al. 2017). We also focus on the dynamical features of order and chaos of some orbits in the system. Then, a post-Newtonian conservative system of compact binaries with one body spinning (Damour et al. 2000a, 2000b, 2001; Nagar 2011) is another tested model in Section 4. Finally, our main results are concluded in Section 5. The extended phase-space explicit methods for inseparable Hamiltonian problems are introduced briefly in the Appendix.

2. A New Energy-conserving Method

Let us consider an $N$-dimensional Hamiltonian problem $H(q, p)$, which corresponds to the following Hamiltonian canonical equations:

$$\dot{q} = \frac{\partial H}{\partial p},$$

$$\dot{p} = -\frac{\partial H}{\partial q}. \tag{1}$$

From an $n$th step to an $(n + 1)$th step, these derivatives have discrete forms:

$$\frac{q_{n+1} - q_n}{\Delta t} = \frac{[H(q_n, p_{n+1}) - H(q_n, p_n)]}{(p_{n+1} - p_n)}, \tag{3}$$

$$\frac{p_{n+1} - p_n}{\Delta t} = \frac{[H(q_n, p_{n+1}) - H(q_{n+1}, p_n)]}{(q_{n+1} - q_n)}. \tag{4}$$

It is easy to obtain from the two equations that

$$H(q_{n+1}, p_{n+1}) - H(q_n, p_n) = 0. \tag{5}$$

That means that the discretized Equations (3) and (4) do exactly conserve the Hamiltonian. Therefore, they are an energy-conserving scheme in the general case. In fact, the discrete gradient is only a discrete average of the Hamiltonian, $\nabla H$. In what follows, we consider how to construct an energy-conserving scheme with a second-order approximation to the gradient of an eight-dimensional Hamiltonian with four degrees of freedom.

Now, let $q$ be a four-dimensional position vector, and $p$ be a four-dimensional momentum vector, i.e., $q = (q_1, q_2, q_3, q_4)$ and $p = (p_1, p_2, p_3, p_4)$. $h = \Delta t$ is a time step. For simplicity, we take the value of $H(q_{1n}, q_{2n}, q_{3n}, q_{4n}, p_{1n}, p_{2n}, p_{3n}, p_{4n})$ at an $n$th step is labeled as $H(00000000)$, and that of $H(q_{1(n+1)}, q_{2(n+1)}, q_{3(n+1)}, q_{4(n+1)}, p_{1(n+1)}, p_{2(n+1)}, p_{3(n+1)}, p_{4(n+1)})$ at an $(n + 1)$th step is marked as $H(11111111)$. In addition, we take $q_{1n} = q_{10}$, $q_{1(n+1)} = q_{11}$, \ldots. Using these notations, we discretize Equations (1) and (2) as follows:

$$\frac{q_{1n} - q_{10}}{h} = \frac{1}{8} \left[ H(00001000) - H(00000000) \right] + \frac{p_{1n} - p_{10}}{h} \right] + \frac{H(00010000) - H(00001000)}{p_{1n} - p_{10}} + \frac{H(00010001) - H(00001001)}{p_{1n} - p_{10}} + \frac{H(00110001) - H(00110001)}{p_{1n} - p_{10}} + \frac{H(00111001) - H(00110001)}{p_{1n} - p_{10}} + \frac{H(00111011) - H(00110011)}{p_{1n} - p_{10}} + \frac{H(01111101) - H(01110101)}{p_{1n} - p_{10}} + \frac{H(01111111) - H(01110111)}{p_{1n} - p_{10}} + \frac{H(11111111) - H(11110111)}{p_{1n} - p_{10}} \right]. \tag{6}$$
\[ \frac{q_{21} - q_{20}}{h} = \frac{1}{8} \left[ \frac{H(00000010) - H(00000000)}{p_{21} - p_{20}} + \frac{H(10001100) - H(10000000)}{p_{21} - p_{20}} + \frac{H(01001100) - H(01000100)}{p_{21} - p_{20}} + \frac{H(10011000) - H(10010000)}{p_{21} - p_{20}} + \frac{p_{21} - p_{20}}{H(10011101) - H(10011011)} \right] \] (7)

\[ \frac{q_{31} - q_{30}}{h} = \frac{1}{8} \left[ \frac{H(00000010) - H(00000000)}{p_{31} - p_{30}} + \frac{H(01000100) - H(01000000)}{p_{31} - p_{30}} + \frac{H(01001100) - H(01000100)}{p_{31} - p_{30}} + \frac{H(10001100) - H(10000100)}{p_{31} - p_{30}} + \frac{H(11001100) - H(11000100)}{p_{31} - p_{30}} + \frac{H(11011110) - H(11011110)}{p_{31} - p_{30}} + \frac{H(11111111) - H(11111111)}{p_{31} - p_{30}} \right] \] (8)

\[ \frac{q_{41} - q_{40}}{h} = \frac{1}{8} \left[ \frac{H(00000001) - H(00000000)}{p_{41} - p_{40}} + \frac{H(00100001) - H(00100000)}{p_{41} - p_{40}} + \frac{H(00100011) - H(00100010)}{p_{41} - p_{40}} + \frac{H(01100011) - H(01100010)}{p_{41} - p_{40}} + \frac{H(01111111) - H(01111111)}{p_{41} - p_{40}} \right] \] (9)

\[ \frac{p_{11} - p_{10}}{h} = \frac{1}{8} \left[ \frac{H(00000000) - H(00000000)}{q_{11} - q_{10}} + \frac{H(01000100) - H(01000100)}{q_{11} - q_{10}} + \frac{H(10011000) - H(10011000)}{q_{11} - q_{10}} + \frac{H(10111100) - H(10111100)}{q_{11} - q_{10}} + \frac{H(11111111) - H(11111111)}{q_{11} - q_{10}} \right] \] (10)

\[ \frac{p_{21} - p_{20}}{h} = \frac{1}{8} \left[ \frac{H(01000000) - H(00000000)}{q_{21} - q_{20}} + \frac{H(01000100) - H(00000100)}{q_{21} - q_{20}} + \frac{H(11001100) - H(10001100)}{q_{21} - q_{20}} + \frac{H(11011100) - H(10111100)}{q_{21} - q_{20}} + \frac{H(11111111) - H(10111111)}{q_{21} - q_{20}} \right] \] (11)
\[
\frac{p_{31} - p_{30}}{h} = -\frac{1}{8} \left[ \frac{H(00100000) - H(00000000)}{q_{31} - q_{30}} \right. \\
+ \frac{H(00100010) - H(00000001)}{q_{31} - q_{30}} \\
+ \frac{H(01100010) - H(01000010)}{q_{31} - q_{30}} \\
+ \frac{H(11100110) - H(11000110)}{q_{31} - q_{30}} \\
+ \frac{H(11111110) - H(11011110)}{q_{31} - q_{30}} \\
\left. + \frac{H(11111111) - H(11011111)}{q_{31} - q_{30}} \right],
\]

(12)

\[
\frac{p_{41} - p_{40}}{h} = -\frac{1}{8} \left[ \frac{H(00000010) - H(00000000)}{q_{41} - q_{40}} \right. \\
+ \frac{H(00010001) - H(00000001)}{q_{41} - q_{40}} \\
+ \frac{H(00110001) - H(00100001)}{q_{41} - q_{40}} \\
+ \frac{H(01101011) - H(01010111)}{q_{41} - q_{40}} \\
+ \frac{H(11101011) - H(11010111)}{q_{41} - q_{40}} \\
\left. + \frac{H(11111111) - H(11011111)}{q_{41} - q_{40}} \right],
\]

(13)

The discretization of each partial derivative of the Hamiltonian with respect to one of the position and momentum variables is the average of eight Hamiltonian difference terms. It is easy to find that the left-hand side of \( \sum_{i=1}^{4} [\text{Equation } (5+i) \cdot (p_{i1} - p_{i0}) - \text{Equation } (9+i) \cdot (q_{i1} - q_{i0})] \) vanishes, and the right-hand side is \( H(11111111) - H(00000000) \)—that is, the discrete Equations (6)–(13) of the Hamiltonian Equations (1) and (2) exactly satisfy the energy-conserving condition (5). These Hamiltonian differencing symmetric forms in the right-hand sides of Equations (6)–(13) possess a second-order accuracy. There is not a systematic method by means of which the difference Equations (6)–(13) have been constructed.

The difference schemes of Equations (6)–(13) for eight-dimensional Hamiltonian problems are not symplectic although they are energy conservative. If Equations (1) and (2) are nonlinear, Equations (6)–(13) should be solved by an iterative method, such as a Newton iterative scheme. However, the iterative solution does not converge when one or more denominators of the right-hand sides in Equations (6)–(13) tend to zero or are sufficiently small. In order to avoid the occurrence of numerical singularities, we should rewrite as much as possible each Hamiltonian difference term so that all same factors between the denominator and the numerator are eliminated in the Hamiltonian difference. If some singularities or sufficiently small denominators still arise, the difference of a certain function is replaced with the partial derivative of the function. More details on how to handle this kind of numerical singularities were provided by Bacchini et al. (2018).

In what follows, we are interested in evaluating the performance of the new energy-conserving (EC) scheme applied to two models. For comparison, an RK method, an implicit midpoint symplectic (IS) method (Feng 1986; Zhong et al. 2010; Mei et al. 2013) and an extended phase-space explicit symplectic-like (ES) integrator (Pihajoki 2015; Liu et al. 2016; Li & Wu 2017; Luo et al. 2017) are employed. The extended phase-space method is simply described in the Appendix.

3. FPU \( \beta \) Lattice

An FPU system (Skokos et al. 2008; Gerlach et al. 2012) with \( N \) dimensions describes the motion of \( N \) particles interaction each other. An FPU \( \beta \) lattice is a perturbed FPU system. For our purpose, we take into account an eight-dimensional FPU \( \beta \) system with four degrees of freedom as follows:

\[
H(q, p) = \sum_{i=1}^{4} \frac{p_{i1}^2}{2} + \sum_{i=0}^{4} \left[ \frac{(q_{i+1} - q_{i})^2}{2} + \beta \frac{(q_{i+1} - q_{i})^4}{4} \right].
\]

(14)

Boundary conditions are \( q_{40} = q_{50} = 0 \), and \( \beta \) is a non-negative parameter.

When the new energy-conserving method EC is applied to this system, its implementation is given here. A key point lies in that singularities or small denominators in the difference terms in the right-hand sides of Equations (6)–(13) should be eliminated as much as possible. For example, the difference term in the right-hand side of Equation (6) is \( [H(00001000) - H(00000000)]/[q_{41} - q_{40}] \). As another example, \( [H(10011000) - H(00011000)]/[q_{41} - q_{40}] = [1 + \beta(q_{41}^2 + q_{40}^2)/2] (q_{41} - q_{40})^2 + (q_{41} + q_{40})^2 - 2q_{40} \) \( (1 + \beta)((q_{41}^2 + q_{40}^2)/2) + (q_{41} + q_{40})^2 - 2q_{40} \) in Equation (10). In this way, all denominators in the right-hand sides of Equations (6)–(13) are no longer present. Hence, with the Newton iterative method the iterative solutions of Equations (6)–(13) acting on the system of Equation (14) have no difficulty.

Taking \( \beta = 1.5 \) and the time step of \( h = 0.01 \), we choose two orbits whose initial conditions are \( q = (0.1, 0.1, 0.2, 0.2) \) for orbit 1, and \( q = (0.1, 0.1, 0.2, 1.1) \) for orbit 2. As shown in Figure 1, the RK method shows a secular growth in the Hamiltonian error, but the new method EC, the implicit symplectic method IS and the extended phase-space method ES do not. The latter three methods make the energy stable. In this sense, they are regarded as energy-conserving schemes. As to the numerical accuracy of the energy, the RK method is the worst, the IS and ES integrators are almost the same, and the
new algorithm EC is the best. In particular, the energy error is smaller in several orders for EC than for IS or ES. It is clear that the new energy-conserving method is greatly superior to both the implicit symplectic method and the extended phase-space method in the conservation of the Hamiltonian.

Figures 1(a) and (b) show that the energy error of orbit 1 given by the new method EC is two orders less than that of orbit 2. This is due to the two orbits having different dynamical behaviors. The maximum Lyapunov exponents $\lambda$ in Figure 2(a) and the fast Lyapunov indicators $\Lambda$ in Figure 2(b) show the regularity of orbit 1 and the chaoticity of orbit 2. Here, the Lyapunov exponents are calculated in terms of the two-particle method (Wu & Huang 2003). A bounded orbit is chaotic if its Lyapunov exponent tends to a stabilized positive value but is regular when the maximum Lyapunov exponent is zero. The fast Lyapunov indicators are also based on the idea of the two-particle method (Wu et al. 2006). If this indicator grows in a power law with time $\log_{10}t$, the bounded orbit is ordered. However, it is chaotic if this indicator grows in an exponential law. According to these criteria for the Lyapunov exponents and the fast Lyapunov indicators distinguishing between the two cases of order and chaos, we can easily determine the dynamical features of orbits 1 and 2 in Figures 2(a) and (b).

Note that the energies of orbits 1 and 2 are 0.031 and 1.815, respectively. This shows that chaos occurs easily for a large energy. Using the newly proposed algorithm through many numerical tests, we find that under the present circumstances, chaos is absent for the energy smaller than 0.5, whereas it is present for the energy larger than 0.5. Table 1 and Figure 3 relate to the regularity and chaoticity of some orbits.

4. Post-Newtonian Hamiltonian of Compact Binaries with One Body Spinning

Various orbits in a post-Newtonian Hamiltonian of compact binaries with one body spinning are used to test the numerical performance of the new algorithm. These orbits include circular, spherical, quasi-spherical, and eccentric orbits.

4.1. Dynamical Model

Since the novel algorithm is only limited to the use of eight-dimensional systems, we consider a compact binary system in which only one body spins. This system consists of two black holes with masses $m_1$ and $m_2$. The total mass is $M = m_1 + m_2$. We take a reduce mass of $\mu = m_1m_2/M$, a mass ratio of $\gamma = m_1/m_2$, and a mass parameter of $\eta = \mu/M = \gamma/(1 + \gamma)^2$. $r = (x, y, z)$ is a coordinate of body 1 relative to body 2, and $n = r/r$ is a radial unit vector, where $r = |r|$ is a radius. We suppose that the spin motion of body 1 is described by $S_1$. The speed of light, $c$, and the constant of gravity, $G$, are one geometric unit, $c = G = 1$. The dynamics of compact binaries can be described by the following post-Newtonian
Spin effects have spin–orbit couplings of $H_{so}(r, p, S_i)$ and spin–spin couplings of $H_{ss}(r, S_i)$. The two types of spin contributions are written as

$$H_{so} = \frac{\eta}{r^3} \left( g_{\alpha} + \frac{1}{\gamma} g_{\beta} \right) S_i \cdot L, \quad (20)$$

$$H_{ss} = \frac{\eta}{2r^7} [3(S_i \cdot n)^2 - S_i^2], \quad (21)$$

$$g_{\alpha} = 2 + \left[ \frac{19}{8} \eta p^2 + \frac{3}{2} \eta (n \cdot p)^2 - (6 + 2\eta) \frac{1}{r} \right], \quad (22)$$

$$g_{\beta} = \frac{3}{2} - \left( \frac{5}{8} + 2\eta \right) p^2 + \frac{3}{4} \eta (n \cdot p)^2 - \frac{1}{r}(5 + 2\eta), \quad (23)$$

$$S_{\gamma} = \left( 1 + \frac{1}{\gamma} \right) S_i, \quad (24)$$

$$L = r \times p. \quad (25)$$

Here, the spin–orbit couplings have 1.5pn and 2.5pn terms and the spin–spin couplings are at the 2pn order. The Newton–Wigner–Pyce spin supplementary condition $\kappa = 0$ (Mikóczi 2017) is used. In addition, the Hamiltonian (15) uses dimensionless operations: $r \rightarrow Mr, \ t \rightarrow Mt, \ H \rightarrow \mu H, \ L \rightarrow \mu L,$ and $S_i \rightarrow \mu S_i$, i.e.,

$$S_i = \hat{S}_i, \ \hat{S}_i = \frac{\chi_i m_i^2}{\mu M}. \quad (26)$$

$\chi_i$ is a dimensionless parameter given at the interval [0, 1], and $\hat{S}_i$ is a unit spin vector.

The position and momentum variables, $r$ and $p$, are conjugate because they satisfy the Hamiltonian canonical Equations (1) and (2). However, the spin variable, $S_i$, is not because its evolution equation is a non-canonical equation

$$\frac{dS_i}{dt} = \frac{\partial H}{\partial S_i} \times S_i. \quad (27)$$

In this case, the application of the new algorithm of Equations (6)–(13) to the system (15) becomes difficult. This problem can be solved with the aid of the canonical, conjugate

**Table 1**

Dynamical Features of Several Orbits in the FPU-β System

| Orbit | Initial Position | $E$ | Dynamics |
|-------|------------------|-----|----------|
| 1     | (0.1, 0.1, 0.2, 0.2) | 0.031 | order |
| 2     | (0.1, 0.1, 0.2, 1.1) | 1.815 | chaos |
| 3     | (0.5, 0.5, 0.5, 0.5) | 0.297 | order |
| 4     | (0.55, 0.5, 0.5, 0.5) | 0.335 | order |
| 5     | (0.6, 0.5, 0.5, 0.5) | 0.382 | order |
| 6     | (0.62, 0.5, 0.5, 0.5) | 0.403 | order |
| 7     | (0.7, 0.5, 0.5, 0.5) | 0.504 | chaos |
| 8     | (0.75, 0.5, 0.5, 0.5) | 0.581 | chaos |
| 9     | (0.8, 0.5, 0.5, 0.5) | 0.670 | chaos |
| 10    | (0.85, 0.5, 0.5, 0.5) | 0.772 | chaos |

Note. These orbits have the same initial momentum of $p = (0, 0, 0, 0)$ but different positions of $q = (q_1, q_2, q_3, q_4)$. $E = H$ corresponds to the energy of each orbit.
spin cylindrical-like coordinates $\theta$ and $\xi$ constructed by Wu & Xie (2010):

$$S_1 = (\rho \cos \theta, \rho \sin \theta, \xi\gamma), \quad \rho = \sqrt{S_1^2 - \xi^2}. \quad (28)$$

It is clear that $S_1$ is a two-dimensional vector with three components. The Hamiltonian (15) is completely canonical and has eight-dimensional phase-space variables, $q^b = (q, \theta)$ and $p^b = (p, \xi)$. This canonical system is labeled as

$$\mathcal{H}(q^b, p^b) = \mathcal{H}(q, p, S_1), \quad (29)$$

which has four independent integrals: the total energy (i.e., $\mathcal{H}$) and three components of the total angular momentum vector, $J = L + S_1$. Therefore, $\mathcal{H}$ is integrable and non-chaotic.

4.2. Numerical Investigations

Without doubt, the new energy-conserving algorithm given by Equations (6)–(13) is suitable for the canonical system $\mathcal{H}$ in Equation (29). Problems of numerical singularities or small denominators may frequently occur but can be solved in terms of the suggestions given in Section 2.

Taking the parameters $\chi = 1, \gamma = 1$ and initial conditions $y = z = p_x = p_y = 0, \theta = \xi = 0$ and $p_z = \sqrt{(1 - \varepsilon)/\varepsilon}$, we plot Figure 4(a) in which the Hamiltonian errors of the above algorithms solving orbit 1 in Table 2 are shown. The new method EC, the implicit symplectic integrator IS, and the extended phase-space method ES can make the Hamiltonian errors stable. The energy error for EC is of the order of $10^{-15}$, and those for IS and ES remain of the order of $10^{-6}$. The energy error for RK increases with time and reaches an order of $10^{-5}$ when the Hamiltonian errors of the above algorithms solving orbit 1 in Table 2 are shown. These results are what we expect and seem to be independent of the initial eccentricity, $e$. See Table 2 for more information. The results are obtained from large initial orbital radii and different time steps. For a small initial radius and a fixed time step, e.g., $r = x = 40$ and $h = 0.1$ in Table 3, these algorithms that act on some orbits show a similar performance. Of course, there are some differences. The energy errors for the three methods, RK, IS, and ES, are closely associated to the initial eccentricity and become large with the increasing eccentricity, but the energy error for the new scheme EC is not very sensitive dependent on the initial eccentricity and still remains of the order of $10^{-14}$ after the integration time $10^5$. These results in Tables 2 and 3 are given when the spin–orbit couplings and spin–spin effects are included together. What about relative position errors of these algorithms? When more accurate solutions given by an eighth- and ninth-order Runge–Kutta–Fehlberg algorithm of variable step sizes are taken as reference solutions, the relative position errors that these methods show can be obtained in Figure 4(b). As the integration times are long enough and a larger time step is adopted, the position errors remain stable for the new method EC, whereas they grow with time for the other three methods. Particularly for the RK method, its position errors are larger than for EC after a long enough time.

It is not only at the starting time but also at any time that the eccentricity of orbit 10 in Table 3 is always identical to zero in Equation (16) when no body spins. In fact, this orbit is an exact circular orbit. This is because it satisfies the conditions of circular orbits on the equatorial plane: $dr/dt = \partial H_o/\partial p_y = 0$, $p_r = 0$, and $\partial H_o/\partial r = 0$, where $p_r = n \cdot p$ denotes a radial momentum. In this case, $p^2 = p_z^2 + L^2/r^2 = L^2/r^2$, where $L_r = xp_r = 6.6473$ is the $z$ component of the orbital angular momentum, $L$. The angular frequency of the circular orbit is $\omega_z = \partial H_o/\partial L_r = 0.0038$. Such a circular orbit is used to check the numerical performance of these methods. Because this orbit is only limited to staying at a six-dimensional phase space of the system in Equation (16), the energy-conserving method of Bacchini et al. (2018) rather than the new energy-conserving scheme is suitable for integrating this orbit. The four methods give the energy errors (not plotted) to the circular orbit, like those to orbit 1 in Figure 4(a). They almost remain of the radius $r = 40$ of the circular orbit in Figure 5(a) when the integration times are short. However, the position errors for RK will be larger than for the EC method as the integration times last long enough in Figure 5(b). This result looks like that of orbit 1 in Figure 4(b). The EC method does not show a secular growth in the position errors in Figures 4(b) and 5(b). Of course, there is a typical difference between Figures 4(b) and 5(b) that the implicit symplectic integrator IS and the extended phase-space method ES have a secular growth in the position errors of orbit 1 but do not have in the position errors of the circular orbit. When the spin–orbit couplings in Equation (20) are added to the orbital part (16),...
the term $H_{\text{so}}$ is a conserved quantity and does not contain $p_r$. Therefore, $dr/dt = 0$ is still existent. The radius $r = 40$ remains invariant, but the orbit is a spherical orbit rather than a circular orbit because of the spin of body 1 leading to the precession of orbits. This spherical orbit with the angular frequency $\omega_{\text{so}} = \omega_{\text{so}} + \partial H_{\text{so}}/\partial L_z = 0.0038$ is an orbit in a eight-dimensional phase space and so our new EC method rather than the energy-conserving method of Bachini et al. (2018) becomes useful. The four algorithms show the preference of such a spherical orbit during a short integration time in Figure 5(c). The position errors in Figure 5(d) are also similar to those in Figure 5(b). A difference lies in that the position errors are smaller for RK than for EC. When the spin–spin interactions in Equation (21) are also included, these methods almost give same Figure 5(e) that the radius $r$ oscillates around 40.025 in a small amplitude and the spherical orbit is slightly destroyed. This destruction of the spherical orbit is not large because the spin–spin effects are small compared to the spin–orbit ones. With the inclusion of the spin–spin couplings, the spherical orbit yielded by the spin–orbit couplings becomes a quasi-spherical orbit. The position errors given by these schemes for the quasi-spherical orbit in Figure 5(f) are almost the same as those for the spherical orbit in Figure 5(d). If the time step $h = 1$ in Figure 5 is replaced with a small time step $h = 0.01$ in Table 4, the relative position errors are the smallest for ES but the largest for EC. RK and IS have almost the same errors.

Now, let eccentrical orbits (e.g., the eccentric orbit 11 in Table 3) be used as tested orbits. For this case, the energy errors (not plotted) that the four algorithms show are nearly the same as those in Figure 4(a). The relative position errors have secular growths for the four algorithms, as shown in Figure 6. They are larger for RK than for EC after a long enough time. Seen from the above numerical experiments, the new method is the most effective to conserve energies compared to the other three schemes. However, it is not superior to the RK method in the accuracy of numerical solutions when the time step is small and the integration time is not long enough, as shown in Figures 4(b), 5(b), (d), (f), and 6 and Table 4. In other words, such energy-conserving integrators are typically characterized by larger trajectory errors. This is because numerical errors that are prevented in the energy are then reversed to the position. For periodic or bounded motion, such errors can be typically ignored, since they will mostly result in frequency/phase mismatches without causing the disruption of the bounded orbit. On the other hand, the energy-conserving integrators are nonsymplectic, hence they are not characterized by conservation of phase-space trajectories. The highly geometric character of these integrators suffices in preserving phase-space trajectories to a high degree. It is, however, not impossible that some geometric features of the trajectory may suffer from additional numerical errors, which would be absent in symplectic integrators. Besides this drawback, the energy-conserving integrators need much additional computational cost, since they are implicit and involve a system of nonlinear equations that are handled during the computation. This fact is confirmed in Table 5.

### Table 2

| Orbit | $x$ | $e$ | $h$ | EC | RK | ES | IS |
|-------|-----|-----|-----|----|----|----|----|
| 1     | 120 | 0.0 | 15  | $8.37 \times 10^{-16}$ | $2.83 \times 10^{-6}$ | $1.53 \times 10^{-8}$ | $3.05 \times 10^{-8}$ |
| 2     | 120 | 0.1 | 5   | $6.79 \times 10^{-16}$ | $2.47 \times 10^{-7}$ | $3.23 \times 10^{-9}$ | $6.46 \times 10^{-9}$ |
| 3     | 120 | 0.2 | 10  | $3.77 \times 10^{-16}$ | $5.77 \times 10^{-8}$ | $1.95 \times 10^{-8}$ | $3.33 \times 10^{-8}$ |
| 4     | 120 | 0.35| 4   | $9.92 \times 10^{-16}$ | $2.06 \times 10^{-5}$ | $2.78 \times 10^{-8}$ | $6.46 \times 10^{-8}$ |
| 5     | 120 | 0.55| 5   | $2.68 \times 10^{-15}$ | $1.33 \times 10^{-5}$ | $2.64 \times 10^{-6}$ | $5.66 \times 10^{-9}$ |
| 6     | 120 | 0.6 | 5   | $3.13 \times 10^{-15}$ | $6.71 \times 10^{-7}$ | $1.48 \times 10^{-6}$ | $2.90 \times 10^{-6}$ |
| 7     | 120 | 0.65| 5   | $2.88 \times 10^{-15}$ | $3.31 \times 10^{-9}$ | $3.51 \times 10^{-11}$| $1.20 \times 10^{-10}$|
| 8     | 120 | 0.7 | 5   | $5.74 \times 10^{-15}$ | $2.84 \times 10^{-5}$ | $9.36 \times 10^{-10}$| $1.71 \times 10^{-11}$|

Note. The spin–orbit couplings and spin–spin effects are included together. Initial values of $x$ and $e$ are given below, $py = \sqrt{(1 - e)/x}$, and other initial values are 0. The time step $h$ for each orbit may be different.

### Table 3

| Orbit | $p_y$ | $e$ | EC | RK | ES | IS |
|-------|-------|-----|----|----|----|----|
| 10    | 0.166 | 0.0 | $6.03 \times 10^{-16}$ | $1.34 \times 10^{-10}$ | $2.88 \times 10^{-14}$ | $5.71 \times 10^{-14}$ |
| 11    | 0.158 | 0.0 | $5.07 \times 10^{-15}$ | $5.27 \times 10^{-10}$ | $2.08 \times 10^{-10}$ | $4.16 \times 10^{-10}$ |
| 12    | 0.141 | 0.2 | $2.07 \times 10^{-15}$ | $2.31 \times 10^{-9}$  | $1.27 \times 10^{-9}$  | $2.55 \times 10^{-9}$  |
| 13    | 0.122 | 0.4 | $7.74 \times 10^{-15}$ | $4.60 \times 10^{-8}$  | $2.07 \times 10^{-8}$  | $4.15 \times 10^{-8}$  |
| 14    | 0.100 | 0.6 | $6.88 \times 10^{-15}$ | $1.43 \times 10^{-6}$  | $2.73 \times 10^{-6}$  | $5.49 \times 10^{-8}$  |
| 15    | 0.071 | 0.8 | $1.50 \times 10^{-14}$ | $1.19 \times 10^{-5}$  | $7.16 \times 10^{-10}$ | $1.15 \times 10^{-10}$ |

Note. The spin–orbit couplings and spin–spin effects are included together. Initial value of $x = 40$, those of $p_y$ and $e$ are given below, and other initial values including the initial canonical spin cylindrical-like coordinates $\theta$ and $\xi$ are 0. The time step $h = 0.1$ is fixed.
5. Summary

The novel energy-conserving method given by Equations (6)–(13) is specifically designed for an eight-dimensional Hamiltonian system with four degrees of freedom. In this algorithm, eight partial derivatives of the Hamiltonian with respect to each phase-space variable are discretized and the discretization of the partial derivatives is the average of eight Hamiltonian difference terms. This average gives a second-order accuracy to the Hamiltonian derivative. This algorithm is implicit and can be solved with the aid of the Newton iterative method when the Hamiltonian is nonlinear. It is exactly energy conserving from the theoretical viewpoint but is nonsymplectic.

When the FPU-β lattice is chosen as a tested model, the newly proposed method is shown to have extremely good numerical performance in the conservation of energy. Regardless of whether the considered orbit is regular or chaotic, this new algorithm is greatly superior to the RK method, the implicit midpoint symplectic method, and the extended phase-
the preservation of energies regardless of initial orbital model, the newly proposed method is still extremely good in binaries with one body spinning is used as another tested ones in the system. The threshold of energies between order conserving accuracy of the new algorithm is better for the

| Steps | EC | RK | ES | IS |
|-------|----|----|----|----|
| 300   | $6.9 \times 10^{-10}$ | $7.0 \times 10^{-14}$ | $2.0 \times 10^{-14}$ | $3.7 \times 10^{-14}$ |
| 600   | $1.4 \times 10^{-10}$ | $2.8 \times 10^{-13}$ | $7.2 \times 10^{-14}$ | $1.4 \times 10^{-13}$ |
| 900   | $2.1 \times 10^{-9}$ | $6.4 \times 10^{-13}$ | $1.5 \times 10^{-13}$ | $3.2 \times 10^{-13}$ |
| 1800  | $4.6 \times 10^{-9}$ | $2.5 \times 10^{-12}$ | $6.4 \times 10^{-13}$ | $1.3 \times 10^{-12}$ |
| 2000  | $5.2 \times 10^{-9}$ | $3.1 \times 10^{-12}$ | $7.9 \times 10^{-13}$ | $1.6 \times 10^{-12}$ |

Spherical Orbit

| Steps | EC | RK | ES | IS |
|-------|----|----|----|----|
| 300   | $3.4 \times 10^{-10}$ | $7.0 \times 10^{-14}$ | $2.0 \times 10^{-14}$ | $3.7 \times 10^{-14}$ |
| 600   | $6.0 \times 10^{-10}$ | $2.8 \times 10^{-13}$ | $7.2 \times 10^{-14}$ | $1.4 \times 10^{-13}$ |
| 900   | $7.8 \times 10^{-10}$ | $6.4 \times 10^{-13}$ | $1.6 \times 10^{-13}$ | $3.2 \times 10^{-13}$ |
| 1800  | $6.0 \times 10^{-13}$ | $2.5 \times 10^{-12}$ | $6.4 \times 10^{-13}$ | $1.3 \times 10^{-12}$ |
| 2000  | $5.4 \times 10^{-10}$ | $3.1 \times 10^{-12}$ | $7.9 \times 10^{-13}$ | $1.6 \times 10^{-12}$ |

Quasi-spherical Orbit

| Steps | EC | RK | ES | IS |
|-------|----|----|----|----|
| 300   | $3.4 \times 10^{-10}$ | $7.0 \times 10^{-14}$ | $1.7 \times 10^{-14}$ | $3.5 \times 10^{-14}$ |
| 600   | $6.1 \times 10^{-10}$ | $2.8 \times 10^{-13}$ | $7.5 \times 10^{-14}$ | $1.4 \times 10^{-13}$ |
| 900   | $7.8 \times 10^{-10}$ | $6.4 \times 10^{-13}$ | $1.7 \times 10^{-13}$ | $3.2 \times 10^{-13}$ |
| 1800  | $7.9 \times 10^{-12}$ | $2.5 \times 10^{-12}$ | $6.4 \times 10^{-13}$ | $1.3 \times 10^{-12}$ |
| 2000  | $5.3 \times 10^{-10}$ | $3.1 \times 10^{-12}$ | $7.9 \times 10^{-13}$ | $1.6 \times 10^{-12}$ |

Note. Here, the time step $h = 0.01$ is unlike the time step $h = 1$ in Figures 5(b), (d), and (f).

Table 4
Relative Position Errors for the Four Algorithms that Solve the Circular, Spherical, and Quasi-spherical Orbits in Figure 5

Table 5
CPU Times (Unit: Seconds) for the Four Methods Solving Various Orbits with Different Time Steps $h$

| Orbit | $h$ | EC | RK | ES | IS |
|-------|-----|----|----|----|----|
| 1     | 15  | 59 | 1  | 1  | 2  |
| 2     | 5   | 176 | 3  | 4  | 6  |
| 3     | 10  | 86  | 1  | 2  | 3  |
| 4     | 4   | 214 | 3  | 5  | 7  |
| 5     | 5   | 171 | 3  | 4  | 6  |
| 6     | 5   | 172 | 3  | 4  | 6  |
| 7     | 8   | 107 | 2  | 2  | 4  |
| 8     | 2   | 428 | 6  | 9  | 13 |
| 9     | 2.5 | 342 | 5  | 8  | 11 |
| 10    | 0.1 | 905 | 13 | 19 | 25 |
| 11    | 0.1 | 918 | 13 | 19 | 25 |
| 12    | 0.1 | 890 | 13 | 19 | 25 |
| 13    | 0.1 | 866 | 13 | 19 | 26 |
| 14    | 0.1 | 841 | 13 | 19 | 27 |
| 15    | 0.1 | 848 | 13 | 19 | 27 |

Note. The integration times are $t = 10^6$ for orbits 1–9 and $t = 10^5$ for orbits 10–15.

large time steps compared to the state-of-the-art RK method in the accuracy of numerical solutions. It exhibits a higher computational cost than any one of the other three algorithms.

For some specific purposes on the preservation of energies in numerical simulations with much longer times, such energy-conserving integrators are worth recommending for application. The new integrator could be used to simulate relativistic charged particles moving in a time-varying external electromagnetic field (Pétrí 2017). Such a field can be described by an associated time-dependent Hamiltonian. This Hamiltonian $H$ has eight dimensions, including three spatial coordinates $+ \text{ time}$, three velocity components, and time change with respect to proper time (i.e., the Lorentz factor). By extending the phase space of the Hamiltonian, we will obtain a zero Hamiltonian $\hat{H} = H + p_0$, where $p_0$ is a momentum with respect to time. This would provide a mean to simulate charged particles in time-varying external fields with exact zero-Hamiltonian conservation, which is a very desirable feature in the context of test particle simulations in high-energy astrophysical scenarios. The new integrator will also be suitable for modeling a time-dependent spacetime (Bohn et al. 2015). Although the Hamiltonian $H = \frac{1}{2}g_{\alpha \beta}p_\alpha p_\beta$ for the spacetime, $dS^2 = g_{\alpha \beta}dx^\alpha dx^\beta$, does explicitly depend on the coordinate time, $t$, it has an invariant quantity, $H = -1/2$. From the theory, this invariant quantity can still be preserved by the new integrator. With the aid of the integrator, the characteristic of gravitational waves for circular, spherical, quasi-spherical, and eccentric orbits in relativistic post-Newtonian systems of compact binaries will be analyzed in the future work.

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4 The purposes, e.g., are to obtain higher accuracies of the semimajor axis, mean motion, and mean anomaly in the Keplerian problem in the solar system or to accurately grasp the frequency of a gravitational wave emitted from the circular, spherical, or quasi-spherical orbit in relativistic post-Newtonian systems of compact binaries.
Appendix

Extended Phase-space Explicit Leapfrog Integrators for Inseparable Hamiltonian Problems

Usually, an explicit second-order leapfrog integrator of Wisdom & Holman (1991) is not suitable for Hamiltonian problems with inseparable forms of coordinates and momenta. However, it is still valid if the extended phase-space method of Pihajoki (2015) is considered. Although a Hamiltonian $H(q, p)$ is inseparable, its modified form is

$$\Gamma(q, \dot{q}, p, \dot{p}) = H_1(q, \dot{q}) + H_2(\dot{q}, p),$$

(30)

where $H_1 = H_2 = H$ can be split into two solvable parts, $H_1$ and $H_2$. $A(h)$ is an operator of $H_1$, and $B(h)$ is another operator of $H_2$. The leapfrog algorithm for the new Hamiltonian $\Gamma$ is

$$S(h) = A\left(\frac{h}{2}\right)B(h)A\left(\frac{h}{2}\right).$$

(31)

Under the same initial conditions, the original solution $(q, p)$ and the extended solution $(\tilde{q}, \tilde{p})$ should be the same. However, their coupled derivatives lead to both solutions having some differences. To make the two solutions equal, the leapfrog $S(h)$ needs maps as feedback after the two solutions, e.g.,

$$ES(h) = M \otimes S(h),$$

(32)

where $M$ is a map. These permuted maps can be given in various forms, such as the maps of Pihajoki (2015) and Liu et al. (2016). As a good choice of the map $M$, the midpoint permutations between the old variables $(q, p)$ and the new variables $(\tilde{q}, \tilde{p})$ are given by Luo et al. (2017):

$$\frac{q + \tilde{q}}{2} \rightarrow q,$$

$$\frac{q + \tilde{q}}{2} \rightarrow \tilde{q},$$

$$\frac{p + \tilde{p}}{2} \rightarrow p,$$

$$\frac{p + \tilde{p}}{2} \rightarrow \tilde{p}.$$  

(33)

This algorithm ES is an extended phase-space explicit leapfrog integrator. The inclusion of the permuted map makes this algorithm nonsymplectic. However, this integrator is a symmetric method and shows no secular growth in the errors of energy.

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