

# Secular numerical error in $H = T(p) + V(q)$ symplectic integrator: simple analysis for error reduction

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A simple error analysis for  $H = T(p) + V(q)$  symplectic integrator (i.e. not mixed-variable type) is presented. The truncation error in a second-order integrator is analytically analyzed up to first-order approximation for the two-body problem using a canonical perturbation theory. In  $H = T(p) + V(q)$  type integrators, we cannot employ sophisticated techniques such as warm start or symplectic corrector for the reduction of secular numerical error. But we have confirmed that so-called “iterative start,” where we repeat many short-term numerical integrations while gradually changing initial orbital configuration and searching a point with minimum numerical error, may reduce the secular numerical error in angle variables under certain conditions. According to our numerical integrations on two kinds of three-body planetary systems (weakly and strongly perturbed), simple  $H = T(p) + V(q)$  symplectic integrators are still useful when employed together with the iterative start. To obtain a simple interpretation how the errors are reduced (or not reduced in most systems), we take a nonlinear pendulum system with one degree of freedom for an example, and illustrate that the reduction of the numerical error in  $H = T(p) + V(q)$  symplectic integrator occurs when the potential energy of the system is not an “isochrone” one — when the fundamental frequency of the system depends on initial amplitude of oscillation.

## 1. Introduction

In dynamical studies of solar and extrasolar planetary objects, analytical complexity of perturbation techniques and development of fast computers has led us to the investigation by numerical methods. One of the promising ways for long-term numerical integrations is symplectic integrator designed specifically to maintain the Hamiltonian structure of equations of motion (Yoshida, 1990b; Gladman *et al.*, 1991; Kinoshita *et al.*, 1991; Kinoshita and Nakai, 1992; Yoshida, 1993; Sanz-Serna and Calvo, 1994). One of the typical types of the symplectic integrators splits the Hamiltonian  $H$  into two integrable parts as  $H = T(p) + V(q)$  where  $T$ ,  $V$ ,  $q$ , and  $p$  are kinetic energy, potential energy, canonical coordinate and conjugate momentum, respectively. On the other hand, so called Wisdom-Holman map (also called “mixed variable symplectic integrator,” and hereafter we call it “WH map”) by Wisdom and Holman (1991, 1992) can be more accurate by a factor of the ratio of planetary to central mass than the general-purpose symplectic integrators of  $H = T + V$  type. The principle behind the WH map is to split the Hamiltonian into an unperturbed Kepler part and a perturbation part as  $H = H_{\text{kep}}(L) + H_{\text{int}}(l)$ , where  $L$  and  $l$  denote canonical variables for Keplerian motion symbolically. In each step of the integration, the system is first moved forward in time according to Kepler motion  $H_{\text{kep}}$ , and then a kick in momentum is applied which is derived from the perturbation part of the Hamiltonian,  $H_{\text{int}}$ . Not only the Keplerian part, but also the interaction part is analytical since the perturbation Hamiltonian is basically a function of only relative Cartesian coordinates. The coordinate transformation between  $L$  in  $H_{\text{kep}}$  and  $l$  in  $H_{\text{int}}$  is efficiently encapsulated using the Gauß’s  $f$ - and  $g$ -functions (cf. Danby, 1992).

Also, there are many peripheral techniques for the WH map for the purpose of reducing its numerical error especially in angle variables. They work mostly owing to the smallness of the perturbed part of Hamiltonian ( $H_{\text{int}}$ ) than Keplerian part ( $H_{\text{kep}}$ ). Saha and Tremaine (1992) have devised a special start-up procedure to reduce the truncation error of angle variables, called “warm start,” utilizing one of the characteristics of Hamiltonian system — existence of adiabatic invariant. They have also invented a symplectic scheme with individual stepsizes (though not variable stepsizes), dividing the whole Hamiltonian into each planet’s Keplerian and perturbation parts (Saha and Tremaine, 1994). Wisdom et al. (1996) found a canonical transformation of variables that eliminates error Hamiltonian and greatly improves the accuracy of symplectic integration. This transformation is expressed in terms of a Lie operator that must be applied before each step, and an inverse transformation at the end of each step. This operation is called “symplectic correction.” Some notes on the dependence of the numerical error on initial starting conditions in the WH-type symplectic integrators is also mentioned in Michel and Valsecchi (1996).

There are also many other variants of and modifications to the WH map for the applications in dynamical astronomy. Those kinds of enhancement in symplectic integrators, especially of the WH map, now enable us to perform very long-term numerical integrations ten to hundred times faster than before. With the WH map, timescale of numerical integrations of solar system planetary orbits have reached the age of the solar system, i.e. 4.5 Gyr (Ito *et al.*, 1996; Duncan and Lissauer, 1998; Ito and Tanikawa, 2002).

Now, let us be back at the general-purpose symplectic integrators,  $H = T(p) + V(q)$  type. For problems proxy to the Keplerian motion, the general-purpose method is less efficient than the WH map is. However, the general-purpose method has their literal advantage, i.e. generality: they can be adapted to general dynamical problems which are far from integrable and whose zeroth order approximate solutions are not known. We can think of many of such far-integrable problems, as we discover more and more extrasolar planetary systems, since many of the extrasolar planetary orbital configurations so far discovered are significantly unlike ours (Boss, 1996; Marcy *et al.*, 2000; Marcy and Butler, 2000). Typical ones are the planetary systems in or around binaries. In such systems where the ratio of interaction Hamiltonian  $H_{\text{int}}$  and Kepler Hamiltonian  $H_{\text{kep}}$  is generally not sufficiently small, we cannot exploit the near-integrability of the system which the WH map requires. Also, it is generally not easy to apply the WH map to situations with a lot of close encounters among particles. Though several variants of the WH map are now proposed to handle such collisional systems (Levison and Duncan, 1994; Mikkola, 1997; Lee *et al.*, 1997; Duncan *et al.*, 1998; Chambers, 1999; Mikkola and Tanikawa, 1999), such symplectic schemes might be highly complicated and lose computational efficiency.

Standing on the above viewpoints, we present in this paper a simple error analysis on the  $T(p) + V(q)$  type symplectic integrator (hereafter we call it “TV method” in contrast to the “WH map”). Since many researches have been already done so far on characteristics of the TV symplectic method, this paper may be in a sense an expository one. Hence, to make the way of the error analysis as transparent and general as possible, we take a few very simple dynamical systems as examples: two-body problem, perturbed three-body problems, harmonic oscillator with low degrees of freedom, and a nonlinear pendulum with one degree of freedom. Most of them are nearly integrable, or even analytical solutions are already known. In the former half

of this manuscript, our approach is somewhat close to Kinoshita et al. (1991)’s one. Thus we have felt it advisable to give more details than would otherwise be necessary. This is also in keeping with the view of this paper as an expository one.

In Section 2., we present a brief review of symplectic integrators, especially of the TV method. In Section 3., we will discuss the error Hamiltonian for a first- and second-order TV symplectic methods for the planar two-body problem. Based on the result obtained in this section, we demonstrate to calculate some analytical expressions of numerical symplectic solutions using a canonical perturbation theory in Section 4.. Particularly in the subsection 4.7, we confirm the dependence of numerical longitudinal error on initial orbital configuration. In certain configurations we can significantly reduce the longitudinal error arising from the symplectic integrator; in other words, the iterative start works. While in most configurations, we cannot. In Section 5., we argue on the way of error reduction in angle variables by the iterative start in the TV method. Demonstrations by some numerical experiments in two kinds of three-body systems are described: One is the orbital motion of a “massive” asteroid perturbed by Jupiter, and the other is the orbital motion of an extrasolar planet orbiting around a binary system, MACHO–97–BLG–41. We also mention slightly the “warm start” and its relationship to the topic in this manuscript. Finally in Section 6., we try to illustrate how the errors are reduced or not reduced in various dynamical systems. To explain this qualitatively, we have taken a few systems with low degrees of freedom as examples. We have so far found that we can possibly reduce the numerical error in TV symplectic method considerably by the iterative start when the potential energy  $V$  of the system is not “isochrone” — when fundamental frequency of the system depends on initial amplitude of oscillation.

## 2. Symplectic integrator

First we present a brief review of the generic type of symplectic integrator.

According to Yoshida (1993), explicit symplectic integrators can be reformulated by the Lie algebra (Neri, 1987). We rewrite the Hamilton equations

$$\frac{dq}{dt} = \frac{\partial H}{\partial p}, \quad \frac{dp}{dt} = -\frac{\partial H}{\partial q}, \quad (1)$$

in the form as

$$\frac{dz}{dt} = \{z, H(z)\}, \quad (2)$$

where  $z = q$  or  $p$ , and the braces  $\{, \}$  stands for the Poisson bracket. When we introduce a differential operator  $D_G$  by

$$D_G F \equiv \{F, G\}, \quad (3)$$

then (2) is rewritten as

$$\frac{dz}{dt} = D_H z, \quad (4)$$

so the formal solution, or the exact time evolution of  $z(t)$  from  $t = 0$  to  $t = \tau$  is given by

$$z(\tau) = \left[ e^{\tau D_H} \right] z(0). \quad (5)$$

For a Hamiltonian of the form

$$H = T(p) + V(q), \quad (6)$$

$D_H = D_T + D_V$  and we have a formal solution

$$z(\tau) = \left[ e^{\tau(A+B)} \right] z(0), \quad (7)$$

where  $A \equiv D_T$  and  $B \equiv D_V$ . Operators  $A, B$  are non-commuting in general.

Kinetic energy  $T(p)$  and potential energy  $V(q)$  are individually integrable, so we can get the exact solutions

$$z_A(\tau) = \left[ e^{\tau A} \right] z_A(0), \quad (8)$$

$$z_B(\tau) = \left[ e^{\tau B} \right] z_B(0). \quad (9)$$

Here we should remark that the time evolution of  $z$  under  $e^{\tau A}$  or  $e^{\tau B}$  keeps the symplecticity of the system. This fact is one of the most essential cores of symplectic integration theory. For example, let us take (8) as an example and see how the symplecticity is kept. The symplectic map (8) is a kind of contact canonical transformation under the Hamiltonian  $T(p)$ . Writing down the canonical equation of motion concerning  $T$ , we have

$$\frac{dq}{dt} = \frac{\partial T(p)}{\partial p}, \quad \frac{dp}{dt} = -\frac{\partial T(p)}{\partial q}. \quad (10)$$

Since  $T(p)$  does not contain  $q$ , we get

$$\frac{dp}{dt} = 0, \quad (11)$$

$$\therefore p = \text{constant}, \quad (12)$$

hence we know that  $T(p)$  is also a constant. This leads us to

$$\frac{dq}{dt} = \frac{\partial T(p)}{\partial p}, \quad (13)$$

is a function of  $p$  and also a constant.

$$\therefore q = Ct + q_0, \quad (14)$$

where  $C$  and  $q_0$  are certain constants. (14) means that a particle in phase-space  $(q, p)$  moves linearly with time having a constant velocity. Such an equi-velocity linear motion in phase-space obviously preserves any volume in phase-space. Then the contact transformation (8) preserves the symplecticity of the system whatever value  $\tau$  has. We can apply the same discussion on the contact transformation (9), leading to the conclusion that (9) preserves the symplecticity of the system. Since a product of two canonical transformations is found to be canonical, a map  $e^{\tau A} e^{\tau B}$  also preserves the symplecticity. This argument is applicable to other systems with any degree of freedom. This fact ensures us the area (or volume) preservation property of symplectic schemes. However, note that this character does not directly lead to the conservation of total energy and total angular momentum of the system in symplectic integration.

Now, what we need is the solution under  $H = T(p) + V(q)$ . But since the operators  $A$  and  $B$  are not commutable, we have to find a product which approximates  $e^{\tau(A+B)}$  to an appropriate order.

There is a formula which exactly answers to our question: Baker-Campbell-Hausdorff (BCH) formula (Dragt and Finn, 1976; Varadarajan, 1974) about a product of two exponential functions of non-commuting operators  $X$  and  $Y$ ; when we write the product as

$$e^X e^Y = e^Z, \quad (15)$$

$Z$  turns out to be as follows according to the BCH formula

$$Z = X + Y + \frac{1}{2}[X, Y] + \frac{1}{12}([X, [X, Y]] + [Y, [Y, X]]) + \frac{1}{24}[X, [Y, [Y, X]]] + \dots, \quad (16)$$

where  $[X, Y] \equiv XY - YX$ . For a first-order symplectic integrator, we can apply the BCH formula to  $e^{\tau(A+B)}$  as

$$e^{\tau D_T} e^{\tau D_V} = e^{\tau D_{\tilde{H}_{1st}}}, \quad (17)$$

and obtain

$$\tilde{H}_{1st} = T + V + \frac{\tau}{2}\{V, T\} + \frac{\tau^2}{12}(\{\{T, V\}, V\} + \{\{V, T\}, T\}) + O(\tau^3). \quad (18)$$

For a second-order symplectic integrator, we obtain

$$e^{\frac{\tau}{2} D_T} e^{\tau D_V} e^{\frac{\tau}{2} D_T} = e^{\tau D_{\tilde{H}_{2nd}}}, \quad (19)$$

where

$$\tilde{H}_{2nd} = T + V + \tau^2 \left( \frac{1}{12} \{\{T, V\}, V\} - \frac{1}{24} \{\{V, T\}, T\} \right) + O(\tau^4). \quad (20)$$

Similarly in general, for an  $n$ -th order symplectic integrator, we find the Hamiltonian  $\tilde{H}_n$  as

$$\tilde{H}_n = H + H_{\text{err}} + O(\tau^{n+1}), \quad (21)$$

where  $H = T(p) + V(q)$  and  $H_{\text{err}} = O(\tau^n)$ . We call hereafter  $\tilde{H}$  the Hamiltonian of a surrogate system. We notice that the error of the total energy ( $\tilde{H} - H$ ) remains of the order of  $H_{\text{err}}$ , i.e.  $\tau^n$ .  $H_{\text{err}}$  is a set of terms which consist of  $n$ -fold Poisson brackets and called error Hamiltonian. Note that rigorous convergence of the series (18)(20)(21) is not guaranteed for general nonlinear systems.

### 3. Error Hamiltonian of the two-body problem

The purpose of this section is to express the error Hamiltonian  $H_{\text{err}}$  in a second-order symplectic integrator (20) as a function of Kepler orbital elements. We need the error Hamiltonian to estimate numerical error by symplectic integration in later sections. We take a planar two-body problem (masses  $m_0$  and  $m_1$  with  $\mu = G(m_0 + m_1)$ ) as an example whose dynamical characteristics is very well known.

The Hamiltonian for a two-body problem is written in the heliocentric coordinates  $(\mathbf{q}, \mathbf{v})$

$$H = \tilde{m} \left( \frac{v^2}{2} - \frac{\mu}{r} \right), \quad (22)$$

where

$$\tilde{m} = \frac{m_0 m_1}{m_0 + m_1}, \quad v = |\mathbf{v}|, \quad r = |\mathbf{q}|,$$

with a set of canonical variables  $(\mathbf{q}, \mathbf{p})$  and  $\mathbf{p} = \tilde{m} \mathbf{v}$ . Without loss of generality, we can consider the factor  $\tilde{m}$  in the right-hand side of (22), the reduced mass of the two-body system, as unity. This is possible because there are three units to be determined for a two-body system to dynamically work: mass, length, and time. The determination of  $\mu$ , semimajor axis  $a$  and the reduced mass  $\tilde{m}$  corresponds to the determination of these three units we use. Thus the Hamiltonian of the two-body problem (22) is reduced to that of a system where a infinitesimally small mass particle orbits around a central mass (say, the Sun) whose mass is  $m_0 + m_1$  as

$$H = \frac{v^2}{2} - \frac{\mu}{r}, \quad (23)$$

with canonical variables  $(\mathbf{q}, \mathbf{v})$ . See Appendix A for more details.

Since the kinetic energy  $T(\mathbf{v}) = v^2/2$  is a function only of canonical momentum  $\mathbf{v}$ , and the potential energy  $V(\mathbf{q}) = -\mu/r$  is a function only of canonical coordinate  $\mathbf{q}$ , it is clear

$$\frac{\partial T(\mathbf{v})}{\partial q_i} = 0, \quad \frac{\partial V(\mathbf{q})}{\partial v_i} = 0, \quad (i = 1, 2) \quad (24)$$

Hence the actual expression of the second-order error Hamiltonian up to  $O(\tau^2)$  approximation becomes from (20)

$$\begin{aligned} \frac{H_{\text{err}}}{\tau^2} &= \frac{1}{12} \{ \{ T(\mathbf{v}), V(\mathbf{q}) \}, V(\mathbf{q}) \} - \frac{1}{24} \{ \{ V(\mathbf{q}), T(\mathbf{v}) \}, T(\mathbf{v}) \} \\ &= \frac{1}{12} \left[ \left( \frac{\partial V}{\partial q_1} \right)^2 \frac{\partial^2 T}{\partial v_1^2} + 2 \frac{\partial V}{\partial q_1} \frac{\partial V}{\partial q_2} \frac{\partial^2 T}{\partial v_1 \partial v_2} + \left( \frac{\partial V}{\partial q_2} \right)^2 \frac{\partial^2 T}{\partial v_2^2} \right] \\ &\quad - \frac{1}{24} \left[ \left( \frac{\partial T}{\partial v_1} \right)^2 \frac{\partial^2 V}{\partial q_1^2} + 2 \frac{\partial T}{\partial v_1} \frac{\partial T}{\partial v_2} \frac{\partial^2 V}{\partial q_1 \partial q_2} + \left( \frac{\partial T}{\partial v_2} \right)^2 \frac{\partial^2 V}{\partial q_2^2} \right]. \end{aligned} \quad (25)$$

We need partial derivatives of the kinetic energy

$$T(\mathbf{v}) = \frac{v_1^2 + v_2^2}{2}, \quad (26)$$

and the potential energy

$$V(\mathbf{q}) = -\frac{\mu}{r} = -\mu (q_1^2 + q_2^2)^{-\frac{1}{2}}, \quad (27)$$

in (25). They become as follows:

$$\frac{\partial T}{\partial v_1} = v_1, \quad \frac{\partial T}{\partial v_2} = v_2, \quad (28)$$

$$\left( \frac{\partial T}{\partial v_1} \right)^2 = v_1^2, \quad \left( \frac{\partial T}{\partial v_2} \right)^2 = v_2^2, \quad (29)$$

$$\frac{\partial^2 T}{\partial v_1^2} = \frac{\partial^2 T}{\partial v_2^2} = 1, \quad (30)$$

$$\frac{\partial^2 T}{\partial v_1 \partial v_2} = 0, \quad (31)$$

$$\frac{\partial V}{\partial q_1} = \mu q_1 (q_1^2 + q_2^2)^{-\frac{3}{2}} = \frac{\mu q_1}{r^3}, \quad \frac{\partial V}{\partial q_2} = \mu q_2 (q_1^2 + q_2^2)^{-\frac{3}{2}} = \frac{\mu q_2}{r^3}, \quad (32)$$

$$\left(\frac{\partial V}{\partial q_1}\right)^2 = \mu^2 q_1^2 (q_1^2 + q_2^2)^{-3} = \frac{\mu^2 q_1^2}{r^6}, \quad \left(\frac{\partial V}{\partial q_2}\right)^2 = \mu^2 q_2^2 (q_1^2 + q_2^2)^{-3} = \frac{\mu^2 q_2^2}{r^6}, \quad (33)$$

$$\frac{\partial^2 V}{\partial q_1^2} = \mu \left( \frac{1}{r^3} - \frac{3q_1^2}{r^5} \right) = \frac{\mu}{r^5} (-2q_1^2 + q_2^2), \quad (34)$$

$$\frac{\partial^2 V}{\partial q_2^2} = \mu \left( \frac{1}{r^3} - \frac{3q_2^2}{r^5} \right) = \frac{\mu}{r^5} (-2q_2^2 + q_1^2). \quad (35)$$

Substituting (28)(29)(30)(31)(32)(33)(34)(34) into (25), we get

$$\begin{aligned} \frac{H_{\text{err}}}{\tau^2} &= \frac{1}{12} \left( \frac{\mu^2 q_1^2}{r^6} + \frac{\mu^2 q_2^2}{r^6} \right) - \frac{1}{24} \left[ v_1^2 \frac{\mu}{r^5} (-2q_1^2 + q_2^2) + 2v_1 v_2 \left( -\frac{3\mu q_1 q_2}{r^5} \right) + v_2^2 \frac{\mu}{r^5} (-2q_2^2 + q_1^2) \right] \\ &= \frac{1}{12} \frac{\mu^2}{r^4} - \frac{1}{24} \frac{\mu}{r^5} (-2v_1^2 q_1^2 + v_1^2 q_2^2 - 6v_1 v_2 q_1 q_2 + v_2^2 q_1^2 - 2v_2^2 q_2^2). \end{aligned} \quad (36)$$

Now, expressing the angular momentum integral  $h$  as

$$\begin{aligned} h^2 &= |\mathbf{q} \times \mathbf{v}|^2 \\ &= (q_1 v_2 - q_2 v_1)^2 \\ &= q_1^2 v_2^2 - 2q_1 q_2 v_1 v_2 + q_2^2 v_1^2. \end{aligned} \quad (37)$$

We know that  $h$  can be also expressed by Kepler orbital elements as

$$h = \sqrt{\mu a (1 - e^2)}. \quad (38)$$

Similarly, the energy integral can be expressed as

$$\frac{v^2}{2} - \frac{\mu}{r} = -\frac{\mu^2}{2h^2} (1 - e^2) \quad (39)$$

$$\therefore v^2 = \frac{2\mu}{r} - \frac{\mu^2}{h^2} (1 - e^2), \quad (40)$$

Using (37), (38) and (40), we can rewrite the quantity in the parentheses in the second term of the right-hand side of (36) as

$$\begin{aligned} &-2v_1^2 q_1^2 + v_1^2 q_2^2 - 6v_1 v_2 q_1 q_2 + v_2^2 q_1^2 - 2v_2^2 q_2^2 \\ &= 3 \left( q_1^2 v_2^2 - 2q_1 q_2 v_1 v_2 + q_2^2 v_1^2 \right) - 2 \left( q_1^2 v_2^2 + q_2^2 v_1^2 + v_1^2 q_1^2 + v_2^2 q_2^2 \right) \\ &= 3h^2 - 2 \left( q_1^2 + q_2^2 \right) \left( v_1^2 + v_2^2 \right) \\ &= 3h^2 - 2r^2 v^2 \\ &= 3\mu a (1 - e^2) - 2r^2 \cdot 2 \left( \frac{\mu}{r} - \frac{\mu^2 (1 - e^2)}{2\mu a (1 - e^2)} \right) \\ &= 3\mu a (1 - e^2) - 4\mu r + \frac{2\mu r^2}{a}. \end{aligned} \quad (41)$$

From (36) and (41), the final form of the error Hamiltonian expressed by the Kepler orbital elements becomes

$$\begin{aligned} H_{\text{err}} &= \frac{\tau^2 \mu^2}{12 r^4} - \frac{\tau^2 \mu}{24 r^5} \left( 3\mu a (1 - e^2) - 4\mu r + \frac{2\mu r^2}{a} \right) \\ &= \frac{\tau^2 \mu^2}{24} \left( \frac{6}{r^4} - \frac{3a(1 - e^2)}{r^5} - \frac{2}{ar^3} \right). \end{aligned} \quad (42)$$

The unperturbed or Keplerian part of Hamiltonian is  $-\frac{\mu^2}{2L^2}$ , so the surrogate Hamiltonian  $\tilde{H}$  in the second-order symplectic integrator ends up with

$$\begin{aligned} \tilde{H} &= H + H_{\text{err}} + O(\tau^4) \\ &= -\frac{\mu^2}{2L^2} + \frac{\tau^2 \mu^2}{24} \left( \frac{6}{r^4} - \frac{3a(1 - e^2)}{r^5} - \frac{2}{ar^3} \right) + O(\tau^4). \end{aligned} \quad (43)$$

Next, let us calculate the secular (i.e. time-averaged) value of the error Hamiltonian (42). To do this, time-averaged values of  $\frac{1}{r^3}$ ,  $\frac{1}{r^4}$ ,  $\frac{1}{r^5}$  are necessary. Using the relationship

$$\frac{dl}{df} = \frac{r^2}{a^2 \sqrt{1 - e^2}}, \quad (44)$$

they can be obtained as follows:

$$\begin{aligned} \left\langle \frac{a^3}{r^3} \right\rangle &= \frac{1}{2\pi} \int_0^{2\pi} \frac{a^3}{r^3} dl \\ &= (1 - e^2)^{-\frac{3}{2}}, \end{aligned} \quad (45)$$

$$\begin{aligned} \left\langle \frac{a^4}{r^4} \right\rangle &= \frac{1}{2\pi} \int_0^{2\pi} \frac{a^4}{r^4} dl \\ &= (1 - e^2)^{-\frac{5}{2}} \left( 1 + \frac{e^2}{2} \right), \end{aligned} \quad (46)$$

$$\begin{aligned} \left\langle \frac{a^5}{r^5} \right\rangle &= \frac{1}{2\pi} \int_0^{2\pi} \frac{a^5}{r^5} dl \\ &= (1 - e^2)^{-\frac{7}{2}} \left( 1 + \frac{3e^2}{2} \right). \end{aligned} \quad (47)$$

Substituting (45)(46)(47) into (42), the secular part of the error Hamiltonian becomes

$$\begin{aligned} \langle H_{\text{err}} \rangle &= \left\langle \frac{\mu^2 \tau^2}{24} \left( \frac{6}{r^4} - \frac{3a(1 - e^2)}{r^5} - \frac{2}{ar^3} \right) \right\rangle \\ &= \frac{\mu^2 \tau^2}{24a^4 \eta^5} \left( 1 + \frac{e^2}{2} \right), \end{aligned} \quad (48)$$

where

$$\eta \equiv \sqrt{1 - e^2}. \quad (49)$$



Now we can calculate  $H_{\text{err}}$  for the first-order symplectic integrator as well. Similar to (20), the error Hamiltonian for the first-order symplectic integrator becomes according to the BCH formula as

$$H_{\text{err,1st}} = \frac{\tau}{2} \{V, T\} + \frac{\tau^2}{12} (\{\{T, V\}, V\} + \{\{V, T\}, T\}) + O(\tau^3). \quad (50)$$

For the first term in right-hand side of (50), we get

$$\begin{aligned} \{V(\mathbf{q}), T(\mathbf{p})\} &= \left( \frac{\partial V}{\partial q_1} \frac{\partial T}{\partial p_1} - \frac{\partial V}{\partial p_1} \frac{\partial T}{\partial q_1} \right) + \left( \frac{\partial V}{\partial q_2} \frac{\partial T}{\partial p_2} - \frac{\partial V}{\partial p_2} \frac{\partial T}{\partial q_2} \right) \\ &= \frac{\partial V}{\partial q_1} \frac{\partial T}{\partial p_1} + \frac{\partial V}{\partial q_2} \frac{\partial T}{\partial p_2} \\ &= \frac{\mu q_1}{r^3} \cdot v_1 + \frac{\mu q_2}{r^3} \cdot v_2 \\ &= \frac{\mu}{r^3} (\mathbf{r} \cdot \mathbf{v}). \end{aligned} \quad (51)$$

Each component of the velocity vector  $\mathbf{v}$  is expressed by the Kepler orbital elements on orbital plane as (Danby, 1992)

$$v_1 = -\frac{an}{\eta} \sin f, \quad v_2 = \frac{an}{\eta} (\cos f + e), \quad (52)$$

with

$$q_1 = r \cos f, \quad q_2 = r \sin f, \quad (53)$$

which leads to

$$\begin{aligned} \mathbf{r} \cdot \mathbf{v} &= q_1 v_1 + q_2 v_2 \\ &= r \cos f \left( -\frac{an}{\eta} \sin f \right) + r \sin f \left( \frac{an}{\eta} (\cos f + e) \right) \\ &= -\frac{anr}{2\eta} \sin 2f + \frac{anr}{2\eta} \sin 2f + \frac{e ar n}{\eta} \sin f \\ &= \frac{e ar n}{\eta} \sin f. \end{aligned} \quad (54)$$

We already knew the components of the second term in right-hand side of (50) by (42) as

$$\{\{T, V\}, V\} = \frac{\mu^2}{r^4}, \quad (55)$$

and

$$\{\{V, T\}, T\} = \frac{\mu}{r^5} \left( 3\mu a (1 - e^2) - 4\mu r + \frac{2\mu r^2}{a} \right). \quad (56)$$

Adding all the relevant terms, we get the final form of the error Hamiltonian up to  $O(\tau^2)$  as

$$\begin{aligned} H_{\text{err,1st}} &= \frac{\tau}{2} \{V, T\} + \frac{\tau^2}{12} (\{\{T, V\}, V\} + \{\{V, T\}, T\}) \\ &= \frac{\tau}{2} \frac{\mu}{r^3} \frac{e ar n}{\eta} \sin f + \frac{\tau^2}{12} \left( \frac{\mu^2}{r^4} + \frac{\mu}{r^5} \left( 3\mu a (1 - e^2) - 4\mu r + \frac{2\mu r^2}{a} \right) \right) \\ &= \frac{\tau \mu e ar n}{2\eta r} \sin f + \frac{\tau^2 \mu^2}{12} \left( -\frac{3}{r^4} + \frac{3a(1 - e^2)}{r^5} + \frac{2}{ar^3} \right). \end{aligned} \quad (57)$$

We can calculate the secular part of  $H_{\text{err},1\text{st}}$  by averaging (57) over the period of mean anomaly. First, as for the term of  $O(\tau)$ ,

$$\begin{aligned}
\left\langle \frac{\tau\mu ean}{2\eta r} \sin f \right\rangle &= \frac{1}{2\pi} \frac{\tau\mu ean}{2\eta} \int_0^{2\pi} \frac{\sin f}{r} dl \\
&= \frac{1}{2\pi} \frac{\tau\mu ean}{2\eta} \int_0^{2\pi} \frac{\sin f}{r} \frac{r^2}{a^2\eta} df \\
&= \frac{1}{2\pi} \frac{\tau\mu ean}{2\eta} \frac{a(1-e^2)}{a^2\eta} \int_0^{2\pi} \frac{\sin f}{1+e\cos f} df \\
&= 0.
\end{aligned} \tag{58}$$

As for the terms of  $O(\tau^2)$ , we can calculate them as in the same way with (48). Hence

$$\begin{aligned}
\langle H_{\text{err},1\text{st}} \rangle &= \left\langle \frac{\tau\mu ean}{2\eta r} \sin f + \frac{\tau^2\mu^2}{12} \left( -\frac{3}{r^4} + \frac{3a(1-e^2)}{r^5} + \frac{2}{ar^3} \right) \right\rangle \\
&= \frac{\mu^2\tau^2}{12} \frac{(1-e^2)^{-\frac{5}{2}}}{a^4} \left[ -3 \left( 1 + \frac{e^2}{2} \right) + 3 \left( 1 + \frac{3e^2}{2} \right) + 2(1-e^2) \right] \\
&= \frac{\mu^2\tau^2}{12} \frac{(1-e^2)^{-\frac{5}{2}}}{a^4} (2+e^2) \\
&= \frac{\mu^2\tau^2}{12a^4\eta^5} (2+e^2).
\end{aligned} \tag{59}$$

Therefore we can proceed the same discussion using the secular error Hamiltonian for the first-order symplectic integrator (59) as well as that for the second-order symplectic integrator (48). In the following discussion we focus on the second-order symplectic integrator, so-called ‘‘leap frog,’’ using the error Hamiltonian (48).

## 4. Analytic solution by a canonical perturbation theory

Based on the result obtained in Section 3., we demonstrate to calculate analytical expressions of symplectic numerical solutions using a canonical perturbation theory. We can apply the treatment in this section to symplectic integrators of any order and to perturbation theory to any order, though it immediately leads to a terrible increase of relevant terms.

### 4.1 Canonical perturbation theory by the Lie transformation

Hori (1966, 1967) has developed a perturbation method with unspecified canonical variables utilizing the Lie transformation, and has presented several sample problems by his method (Hori, 1970; Hori, 1971). Hori’s method is characterized for its explicitness of canonical variables; the bothering inversion of old and new variables after obtaining analytical solution is no longer necessary. This is one of the major differences of Hori’s new method from traditional canonical perturbation theories such as by Delaunay or von Zeipel (cf. von Zeipel 1916, Shniad 1970, Yuasa 1971. Consult textbooks by Boccaletti and Pucacco (1998) or Lichtenberg and Lieberman (1992) for their general introduction). Let us briefly summarize the Hori’s perturbation method before applying it to our problem in the next subsection.

Let  $\xi, \eta$  be a set of  $2n$  canonical variables and  $f(\xi, \eta), S(\xi, \eta)$  be arbitrary functions of  $\xi, \eta$ . Differential operators  $D_s^n (n = 0, 1, 2, \dots)$  are defined as

$$D_s^0 f = f, \quad (60)$$

$$D_s^1 f = \{f, S\}, \quad (61)$$

$$D_s^n f = D_s^{n-1}(D_s^1 f). \quad (n \geq 2) \quad (62)$$

Then, the following theorem is due to Lie (1888): A set of  $2n$  variables  $\mathbf{x}, \mathbf{y}$  defined by the equation

$$f(\mathbf{x}, \mathbf{y}) = \sum_{n=0}^{\infty} \frac{\epsilon^n}{n!} D_s^n f(\xi, \eta), \quad (63)$$

is canonical if the series in the right-hand side of (63) converges.  $\epsilon$  is a small constant independent of  $\xi$  and  $\eta$ .

Let us consider a nearly integrable Hamiltonian system which is described by two-dimensional Delaunay variables  $(L, G, l, g)$  as

$$H(L, G, l, g) = H_0(L) + H_1(L, G, l, g), \quad (64)$$

where  $H_0(L)$  is the integrable part and  $H_1(L, G, l, g)$  is the perturbation part. Then, let us apply the Hori's perturbation method to the Hamiltonian system (64) to obtain the solution of the system. The general policy to apply canonical transformation here is to remove all angles and to make the system be integrable, such as

$$H^*(L^*, G^*) = H_0^*(L^*) + H_1^*(L^*, G^*), \quad (65)$$

where a superscript  $*$  symbolically denotes that the variables (or functions) have been canonically transformed.

As for the zeroth order Hamiltonian, the function form is the same before and after the canonical transformation:

$$H_0^*(L^*) = H_0(L^*). \quad (66)$$

Next we introduce a parameter  $t^*$  which satisfies the following relationship and is removed later on as

$$\frac{dL^*}{dt^*} = -\frac{\partial H_0^*}{\partial l^*}, \quad \frac{dl^*}{dt^*} = \frac{\partial H_0^*}{\partial L^*}, \quad (67)$$

$$\frac{dG^*}{dt^*} = -\frac{\partial H_0^*}{\partial g^*}, \quad \frac{dg^*}{dt^*} = \frac{\partial H_0^*}{\partial G^*}. \quad (68)$$

It is clearly seen that the system  $H_0^*$  is integrable since  $H_0^*$  is a function of only  $L^*$ . Then we get the following solution with constants of integration  $C_1, C_2, C_3$  and  $C_4$  as

$$L^* = C_1, \quad g^* = C_2, \quad G^* = C_3, \quad (69)$$

$$\frac{dl^*}{dt^*} = \frac{\partial H_0^*}{\partial L^*} = \text{constant}, \quad (70)$$

$$\therefore l^* = \text{constant} \times t^* + C_4. \quad (71)$$

As you can see,  $t^*$  is a time-like variable which describes the evolution of the non-perturbed (or integrable) system,  $H_0^*$ .

To the first-order,  $H_1^*$  becomes the  $t^*$ -averaged part of  $H_1$  as

$$H_1^* = \langle H_1(L^*, G^*, l^*, g^*) \rangle = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T H_1(L^*, G^*, l^*, g^*) dt^*, \quad (72)$$

or, if  $H_1$  is a periodic function of  $t^*$ , then

$$H_1^* = \langle H_1(L^*, G^*, l^*, g^*) \rangle = \frac{1}{T_p} \int_0^{T_p} H_1(L^*, G^*, l^*, g^*) dt^*, \quad (73)$$

where  $T_p$  is the period. Fortunately, the error Hamiltonians  $H_{\text{err}}$  we consider here is nearly periodic in most cases of planetary dynamics, so (73) is convenient instead of (72).

In the actual two-body problem, time  $t$  is related only to the mean anomaly  $l$ . Hence  $dt^*$  can be transformed into  $dl^*/n^*$  in (73) as

$$\begin{aligned} H_1^* = \langle H_1(L^*, G^*, l^*, g^*) \rangle &= \frac{1}{2\pi n^*} \int_0^{2\pi} H_1(L^*, G^*, l^*, g^*) dl^* \\ &= H_1^*(L^*, G^*, -, g^*), \end{aligned} \quad (74)$$

where the sign “-” in  $H_1^*$  denotes the absence of a variable  $l^*$  by elimination.

Thus the canonically transformed Hamiltonian  $H^*$  in (65) up to the first-order finally becomes

$$H^*(L^*, G^*, -, g^*) = H_0^*(L^*) + H_1^*(L^*, G^*, -, g^*), \quad (75)$$

using the first-order generating function  $S_1$  to transform  $H$  into  $H^*$

$$S_1(L^*, G^*, l^*, g^*) = \int (H_1(L^*, G^*, l^*, g^*) - H_1^*(L^*, G^*, -, g^*)) dt^*. \quad (76)$$

Higher-order solutions can be obtained by similar ways.

## 4.2 Solution for $L$

Now let us apply the Hori’s method to symplectic integrators. Here we consider that the integrable part of Hamiltonian  $H_0$  in (64) corresponds to  $H = -\frac{\mu^2}{2L^2}$  in (43), and the perturbed part of Hamiltonian  $H_1$  in (64) corresponds to  $H_{\text{err}}$  in (43). Henceforward we use the notation  $H_0$  as the integrable part and  $H_1$  as the perturbed part of Hamiltonian in this section. In summary,

$$\begin{cases} \tilde{H} = H + H_{\text{err}} \cdots (43) \\ \uparrow \quad \quad \uparrow \quad \quad \uparrow \\ H = H_0 + H_1 \cdots (64) \end{cases} \quad (77)$$

Using the Lie transformation (63), we obtain final solutions for  $L, G, l, g$ . As for  $L$  up to the first-order,

$$\begin{aligned} L &= L^* + \{L^*, S_1\} \\ &= L^* + \left( \frac{\partial L^*}{\partial l^*} \frac{\partial S_1}{\partial L^*} - \frac{\partial L^*}{\partial L^*} \frac{\partial S_1}{\partial l^*} + \frac{\partial L^*}{\partial g^*} \frac{\partial S_1}{\partial G^*} - \frac{\partial L^*}{\partial G^*} \frac{\partial S_1}{\partial g^*} \right) \end{aligned}$$

$$\begin{aligned}
&= L^* - \frac{\partial S_1}{\partial l^*} \\
&= L^* - \frac{\partial}{\partial l^*} \int (H_1 - H_1^*) dt^* \\
&= L^* - \frac{1}{n^*} \frac{d}{dt^*} \int (H_1 - H_1^*) dt^* \\
&= L^* - \frac{1}{n^*} (H_1 - H_1^*), \tag{78}
\end{aligned}$$

where  $\frac{\partial}{\partial l^*}$  is replaced by  $\frac{1}{n^*} \frac{d}{dt^*}$  since  $t^*$  affects on  $H_1$  only through  $l^*$ . Note that since the second term of the right-hand side of the analytic solution (78) is a small quantity of first-order, we can replace  $n^*$  by  $n_0$  here.

In (78),  $L^*$  and  $n^*$  are constants which should be determined by their initial conditions (or observation values). Representing the initial conditions by subscript 0 as  $L_0$  and  $l_0$ , we get

$$L_0 = L^* - \frac{1}{n^*} (H_{1,t=0} - H_1^*), \tag{79}$$

$$\therefore L^* = L_0 + \frac{1}{n^*} (H_{1,t=0} - H_1^*), \tag{80}$$

where  $H_{1,t=0}$  is the initial value of  $H_1$  when  $t = 0$ .

Now we can compare the analytic solution of  $L$  (80) with a solution by numerical symplectic integration. Substituting  $L^*$  of (80) into (78), we have plotted the time variation of the analytic solution of  $L$  in Figure 1 together with a solution by numerical symplectic integration using the second-order symplectic integrator. We have chosen the value of stepsize  $\tau$  as 1/100 of the orbital period  $T$ , i.e.  $\tau/T = 0.01$ . Initial conditions of the two-body system are listed in Table 1. The analytical solution by (78) and the numerical solution coincide very well within the first-order approximation. A higher order analytical solution will further reduce the difference between these two solutions indicated in the lower panel of Figure 1.

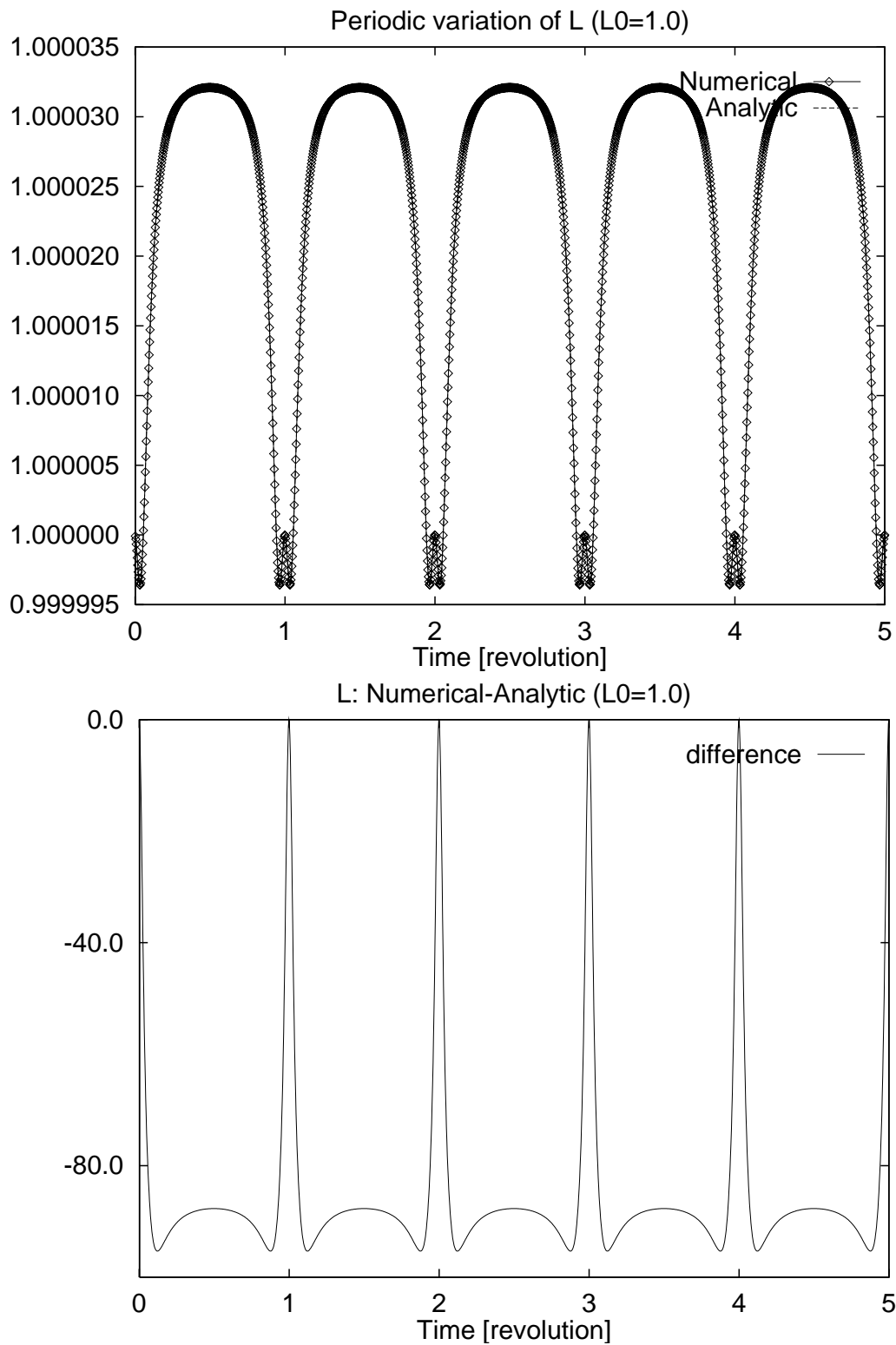
semimajor axis	$a$	1.0
eccentricity	$e$	0.5
argument of pericenter (degrees)	$\omega$	20.0
initial mean anomaly	$l_0$	0.0
mass coefficient	$\mu$	1.0

**Table 1.** Initial conditions for the two-body system used in this section.

Incidentally, from (78) and (80) we obtain

$$\begin{aligned}
L &= L_0 + \frac{1}{n^*} (H_{1,t=0} - H_1^*) - \frac{1}{n^*} (H_1 - H_1^*) \\
&= L_0 + \frac{1}{n^*} (H_{1,t=0} - H_1). \tag{81}
\end{aligned}$$

This means that the secular error of the action  $L$  can be removed up to the first-order by an appropriate selection of the initial value of  $H_1$  so that  $\langle H_{1,t=0} - H_1 \rangle = H_{1,t=0} - H_1^* = 0$ . It is the essential idea of the “iterative start” in Saha and Tremaine (1992) intending to reduce the secular numerical error in the angle  $l$ . We will discuss this fact in later sections.



**Figure 1.** (Upper) analytic and numerical solutions of the Delaunay element  $L$  in the system described in Table 1. The squares denote numerical solution by the second-order symplectic integrator and the lines denote solution by the first-order perturbation theory. (Lower) the difference of the two solutions (numerical – analytical) magnified by  $10^{10}$ .

### 4.3 Solution for $G$

Similar to  $L$ , solution for  $G$  can be obtained up to the first-order as

$$\begin{aligned}
G &= G^* + \{G^*, S_1\} \\
&= G^* + \left( \frac{\partial G^*}{\partial l^*} \frac{\partial S_1}{\partial L^*} - \frac{\partial G^*}{\partial L^*} \frac{\partial S_1}{\partial l^*} + \frac{\partial G^*}{\partial g^*} \frac{\partial S_1}{\partial G^*} - \frac{\partial G^*}{\partial G^*} \frac{\partial S_1}{\partial g^*} \right) \\
&= G^* - \frac{\partial S_1}{\partial g^*} \\
&= G^* - \frac{\partial}{\partial g^*} \int (H_1 - H_1^*) dt^*.
\end{aligned} \tag{82}$$

However, since  $H_1$  does not contain  $g^*$  at all, it becomes

$$\frac{\partial}{\partial g^*} \int (H_1 - H_1^*) dt^* = 0, \tag{83}$$

which means

$$G = G^* = G_0 = \text{constant}. \tag{84}$$

Hence there are no secular nor periodic numerical errors in  $G$  in the second-order symplectic integrator considered here. Actually, it is proved that any type of explicit symplectic integrator rigorously preserves the total angular momentum of system within the range of round-off errors (Yoshida, 1990a; Gladman *et al.*, 1991). In Figure 2, we have plotted relative error of the angular momentum of the two-body system,  $G/G_0 - 1$ , by the symplectic numerical integration. We can see the relative error of  $G$  is very close to the order of the round-off of the computation system,  $O(10^{-16})$ .

### 4.4 Solution for $l$

Same as  $L$  and  $G$ ,

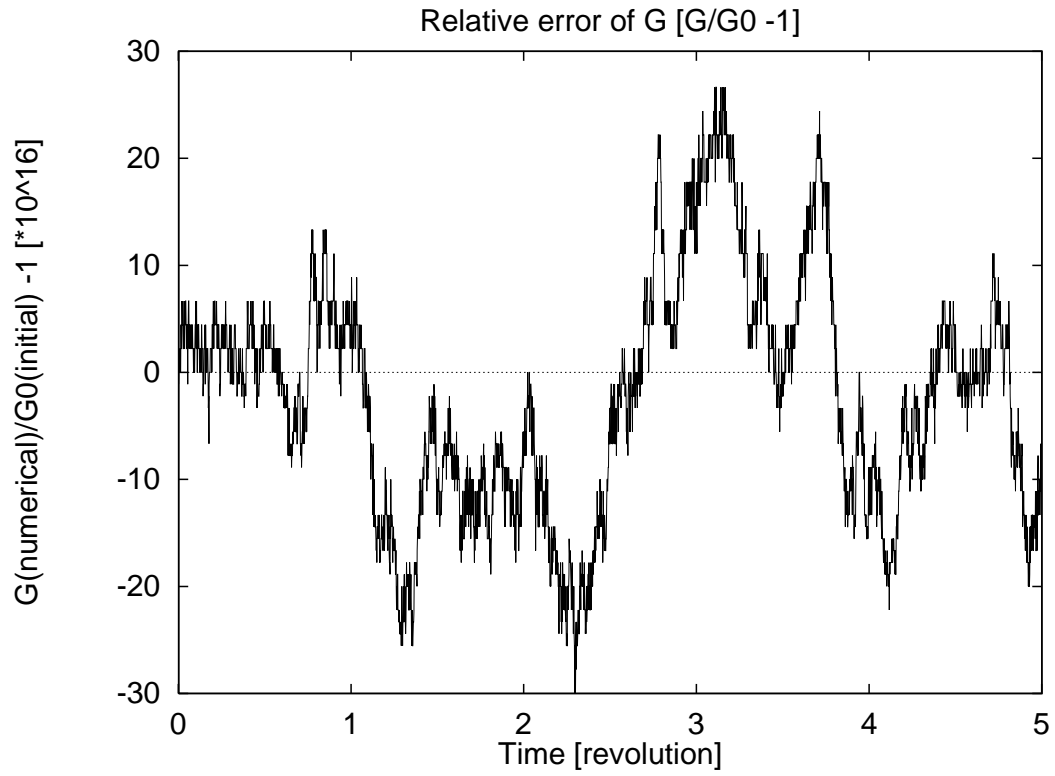
$$\begin{aligned}
l &= l^* + \{l^*, S_1\} \\
&= l^* + \left( \frac{\partial l^*}{\partial l^*} \frac{\partial S_1}{\partial L^*} - \frac{\partial l^*}{\partial L^*} \frac{\partial S_1}{\partial l^*} + \frac{\partial l^*}{\partial g^*} \frac{\partial S_1}{\partial G^*} - \frac{\partial l^*}{\partial G^*} \frac{\partial S_1}{\partial g^*} \right) \\
&= l^* + \frac{\partial S_1}{\partial L^*} \\
&= l^* + \frac{\partial}{\partial L^*} \int (H_1 - H_1^*) dt^*.
\end{aligned} \tag{85}$$

Now the secular error of  $l$  is caused by  $l^*$ , and the periodic error of  $l$  is caused by  $\frac{\partial S_1}{\partial L^*}$ . We show the specific derivation for each of them in the next sections.

#### 4.4.1 Secular error of $l$

The canonical equation of motion on  $l^*$  using the new Hamiltonian (75) is

$$\frac{dl^*}{dt} = \frac{\partial H^*}{\partial L^*}$$



**Figure 2.** The relative error of total angular momentum,  $G/G_0 - 1$ . The quantization around  $10^{-16}$  denotes that the error is due only to round-off because the machine-epsilon of double precision is  $2.2204460492503131 \times 10^{-16}$  in our system (HP-UX 11).



$$\begin{aligned}
&= \frac{\partial}{\partial L^*} \left( -\frac{\mu^2}{2L^{*2}} + \frac{\tau^2 \mu^2}{24a^{*4}\eta^{*5}} \left( 1 + \frac{e^{*2}}{2} \right) \right) \\
&= \frac{\mu^2}{L^{*3}} + \frac{\tau^2 \mu^2}{24} \frac{\partial}{\partial L^*} \left[ a^{*-4} (1 - e^{*2})^{-\frac{2}{5}} \left( 1 + \frac{e^{*2}}{2} \right) \right] \\
&= \frac{\mu^2}{L^{*3}} - \frac{\tau^2 \mu n^*}{12a^{*3}\eta^{*5}} \left( 1 + \frac{5e^{*2}}{4} \right). \quad \left( \because \frac{\mu}{L^*} = \frac{n^{*2}a^{*3}}{n^*a^{*2}} = n^*a^* \right) \tag{86}
\end{aligned}$$

Now we substitute  $L^*$  in (80) into the first term of the right-hand side of (86),

$$\begin{aligned}
\frac{\mu^2}{L^{*3}} &= \frac{\mu^2}{\left( L_0 + \frac{1}{n^*} (H_{1,t=0} - H_1^*) \right)^3} \\
&\simeq \frac{\mu^2}{L_0^3} - \frac{3\mu^2}{L_0^4 n^*} (H_{1,t=0} - H_1^*), \tag{87}
\end{aligned}$$

up to the leading order term of  $H_1/H_0$ .

Therefore (86) becomes

$$\begin{aligned}
\frac{dl^*}{dt} &= \frac{\mu^2}{L_0^3} - \frac{3\mu^2}{L_0^4 n^*} (H_{1,t=0} - H_1^*) - \frac{\mu \tau^2 n^*}{12a^{*3}\eta^{*5}} \left( 1 + \frac{5e^{*2}}{4} \right), \\
&= \frac{\mu^2}{L_0^3} + \tau^2 n^* \left( -\frac{3a^*}{\mu} H_{1,t=0} + \frac{\mu}{24a^{*3}\eta^{*3}} \right). \tag{88}
\end{aligned}$$

$$\therefore l^* = \frac{\mu^2}{L_0^3} t + \tau^2 n^* \left( -\frac{3a^*}{\mu} H_{1,t=0} + \frac{\mu}{24a^{*3}\eta^{*3}} \right) t + l_0. \tag{89}$$

The second term in the right-hand side of (89) represents the secular error of  $l$  up to the first-order of the perturbation theory.

#### 4.4.2 Periodic error of $l$

The periodic error of  $l$  is more complex to calculate. From (85),

$$\begin{aligned}
\frac{\partial S_1}{\partial L^*} &= \frac{\partial}{\partial L^*} \int (H_1 - H_1^*) dt^* \\
&= \frac{\partial}{\partial L^*} \int \left[ \frac{\tau^2 \mu^2}{24} \left( \frac{6}{r^{*4}} - \frac{3a^* (1 - e^{*2})}{r^{*5}} - \frac{2}{a^* r^{*3}} \right) - \frac{\tau^2 \mu^2}{24} \frac{1 + \frac{e^{*2}}{2}}{a^{*4}\eta^{*5}} \right] dt^*. \tag{90}
\end{aligned}$$

It is clear that we have to perform following two calculations successively:

1. Indefinite integration of

$$\int \frac{dt^*}{r^{*n}} = \frac{1}{n^*} \int \frac{dl^*}{r^{*n}}, \quad (n = 3, 4, 5)$$

2. Partial differentiation of the indefinite integrals by  $L^*$ .

Since all the periodic terms are of the first-order, the variables with superscript  $*$  can be replaced by those without  $*$ . We neglect most of the superscripts  $*$  in the following discussion for simplicity.

**Indefinite integrals of  $1/r^{*n}$**  We know relationships between  $r$ ,  $f$ , and  $l$  as

$$r = \frac{a(1-e^2)}{1+e\cos f}, \quad \frac{dl}{df} = \frac{r^2}{a^2\eta}, \quad (91)$$

and the relationships of cosines

$$\cos^2 f = \frac{1}{2}(1 + \cos 2f), \quad \cos^3 f = \frac{1}{4}(\cos 3f + 3\cos f). \quad (92)$$

Using above equations,

$$\begin{aligned} \int \frac{dl}{r^3} &= \int \frac{1}{r^3} \frac{r^2}{a^2\eta} df \\ &= \frac{1}{a^3\eta^3} (f + e\sin f) + \text{constant}, \end{aligned} \quad (93)$$

$$\begin{aligned} \int \frac{dl}{r^4} &= \int \frac{1}{r^4} \frac{r^2}{a^2\eta} df \\ &= \frac{1}{a^4\eta^5} \left[ \left(1 + \frac{e^2}{2}\right) + 2e\sin f + \frac{e^2}{4}\sin 2f \right] + \text{constant}, \end{aligned} \quad (94)$$

$$\begin{aligned} \int \frac{dl}{r^5} &= \int \frac{1}{r^5} \frac{r^2}{a^2\eta} df \\ &= \frac{1}{a^5\eta^7} \left[ \left(1 + \frac{3e^2}{2}\right) f + \left(3e + \frac{3e^3}{4}\right) \sin f + \frac{3e^2}{4}\sin 2f + \frac{e^3}{12}\sin 3f \right] + \text{constant}. \end{aligned} \quad (95)$$

Substituting (93)(94)(95) into (86),

$$\begin{aligned} \int \left( \frac{6}{r^4} - \frac{3a(1-e^2)}{r^5} - \frac{2}{ar^3} \right) dl &= 6 \int \frac{dl}{r^4} - 3a(1-e^2) \int \frac{dl}{r^5} - \frac{2}{a} \int \frac{dl}{r^3} \\ &= \frac{1}{a^4\eta^5} \left[ \left(1 + \frac{e^2}{2}\right) f + \left(e - \frac{e^3}{4}\right) \sin f - \frac{3e^2}{4}\sin 2f - \frac{e^3}{4}\sin 3f \right]. \end{aligned} \quad (96)$$

Hence, the first-order generating function  $S_1$  becomes by (76) with the superscript  $*$  as

$$\begin{aligned} S_1 &= \int (H_1(L^*, G^*, l^*, g^*) - H_1^*) dt^* \\ &= \int \left[ \frac{\tau^2\mu^2}{24} \left( \frac{6}{r^{*4}} - \frac{3a^*(1-e^{*2})}{r^{*5}} - \frac{2}{a^*r^{*3}} \right) - \frac{\tau^2\mu^2}{24} \frac{1 + \frac{e^{*2}}{2}}{a^{*4}\eta^{*5}} \right] dt^* \\ &= \frac{1}{n^*} \int \left[ \frac{\tau^2\mu^2}{24} \left( \frac{6}{r^{*4}} - \frac{3a^*(1-e^{*2})}{r^{*5}} - \frac{2}{a^*r^{*3}} \right) - \frac{\tau^2\mu^2}{24} \frac{1 + \frac{e^{*2}}{2}}{a^{*4}\eta^{*5}} \right] dt^* \\ &= \frac{\tau^2\mu^2}{24n^*a^{*4}\eta^{*5}} \left[ \left(1 + \frac{e^{*2}}{2}\right) f^* + \left(e^* - \frac{e^{*3}}{4}\right) \sin f^* - \frac{3e^{*2}}{4}\sin 2f^* - \frac{e^{*3}}{4}\sin 3f^* - \left(1 + \frac{e^{*2}}{2}\right) l^* \right]. \end{aligned} \quad (97)$$

**Partial derivatives by  $L^*$**  Next we have to calculate the partial derivative  $\frac{\partial S_1}{\partial L^*}$ . All the necessary partial derivatives are given in Appendix C. As for the coefficient part in (97), it becomes (neglecting superscript \*)

$$\frac{\tau^2 \mu^2}{24n^* a^{*4} \eta^{*5}} = \frac{\mu^4}{(\mu a (1 - e^2))^{\frac{5}{2}}} = \frac{\mu^4}{G^5}, \quad (98)$$

Hence

$$\frac{\partial}{\partial L} \frac{\mu^2}{na^4 \eta^5} = \mu^4 \frac{\partial}{\partial L} G^{-5} = 0. \quad (99)$$

Similarly, periodic terms of  $f$  and  $l$  can be differentiated using the relationship

$$\frac{\partial f}{\partial L} = \left( \frac{a}{r} + \frac{L^2}{G^2} \right) \sin f, \quad \frac{\partial l}{\partial L} = 0, \quad (100)$$

as

$$\begin{aligned} \frac{\partial}{\partial L} \left( 1 + \frac{e^2}{2} \right) f &= f \frac{\partial}{\partial L} \left( 1 + \frac{e^2}{2} \right) + \left( 1 + \frac{e^2}{2} \right) \frac{\partial f}{\partial L} \\ &= \frac{G^2}{L^3} f + \frac{G^2}{eL^3} \left( \frac{a}{r} + \frac{L^2}{G^2} \right) \sin f, \end{aligned} \quad (101)$$

$$\begin{aligned} \frac{\partial}{\partial L} \left( e - \frac{e^3}{4} \sin f \right) &= \sin f \frac{\partial}{\partial L} \left( e - \frac{e^3}{4} \right) + \left( e - \frac{e^3}{4} \right) \cos f \frac{\partial f}{\partial L} \\ &= \frac{G^2}{eL^3} \left[ \left( 1 - \frac{3e^2}{4} \right) \sin f + \left( e - \frac{e^3}{4} \right) \left( \frac{a}{r} + \frac{L^2}{G^2} \right) \sin f \cos f \right], \end{aligned} \quad (102)$$

$$\begin{aligned} \frac{\partial}{\partial L} \left( e^2 \sin 2f \right) &= \sin 2f \frac{\partial}{\partial L} e^2 + e^2 \cdot 2 \cos 2f \frac{\partial f}{\partial L} \\ &= \frac{G^2}{eL^3} \cdot 2e \left[ \sin 2f + e \left( \frac{a}{r} + \frac{L^2}{G^2} \right) \cos 2f \sin f \right], \end{aligned} \quad (103)$$

$$\begin{aligned} \frac{\partial}{\partial L} \left( e^3 \sin 3f \right) &= \sin 3f \frac{\partial e^3}{\partial L} + e^3 \cdot 3 \cos 3f \frac{\partial f}{\partial L} \\ &= \frac{G^2}{eL^3} \cdot 3e^2 \left[ \sin 3f + e \left( \frac{a}{r} + \frac{L^2}{G^2} \right) \cos 3f \sin f \right], \end{aligned} \quad (104)$$

$$\begin{aligned} \frac{\partial}{\partial L} \left( 1 + \frac{e^2}{2} \right) l &= l \frac{\partial}{\partial L} \left( 1 + \frac{e^2}{2} \right) \\ &= \frac{G^2}{L^3} l. \end{aligned} \quad (105)$$

Adapting (99)(101)(102)(103)(104) (105) for (97), we get the partial derivative of  $S_1$  by  $L$  (or  $L^*$ ) as

$$\begin{aligned}
\frac{\partial S_1}{\partial L} &= \frac{\tau^2 \mu^2}{24na^4 \eta^5} \left[ \frac{G^2}{L^3} f + \frac{G^2}{eL^3} \left( \frac{a}{r} + \frac{L^2}{G^2} \right) \sin f \right. \\
&\quad + \frac{G^2}{eL^3} \left\{ \left( 1 - \frac{3e^2}{4} \right) \sin f + \left( e - \frac{e^3}{4} \right) \left( \frac{a}{r} + \frac{L^2}{G^2} \right) \sin f \cos f \right\} \\
&\quad - \frac{3}{4} \frac{G^2}{eL^3} \cdot 2e \left\{ \sin 2f + e \left( \frac{a}{r} + \frac{L^2}{G^2} \right) \sin f \cos 2f \right\} \\
&\quad \left. - \frac{1}{4} \frac{G^2}{eL^3} \cdot 3e^2 \left\{ \sin 3f + e \left( \frac{a}{r} + \frac{L^2}{G^2} \right) \sin f \cos 3f \right\} - \frac{G^2}{L^3} l \right] \\
&= \frac{\tau^2 \mu^2}{24na^4 \eta^5} \left[ \frac{G^2}{L^3} (f - l) + \frac{G^2}{eL^3} \left\{ \left( 1 - \frac{3e^2}{4} \right) \sin f + \left( e - \frac{e^3}{4} \right) \left( \frac{a}{r} + \frac{L^2}{G^2} \right) \sin f \right. \right. \\
&\quad + \left( 1 + \frac{e^2}{2} \right) \left( \frac{a}{r} + \frac{L^2}{G^2} \right) - \frac{3}{4} \cdot 2e \left( \sin 2f + e \left( \frac{a}{r} + \frac{L^2}{G^2} \right) \cos 2f \right) \\
&\quad \left. \left. - \frac{1}{4} \cdot 3e^2 \left( \sin 3f + e \left( \frac{a}{r} + \frac{L^2}{G^2} \right) \cos 3f \right) \right\} \right]. \tag{106}
\end{aligned}$$

Therefore, from (85) and (89), the final solution for  $l$  up to the first-order perturbation in this theory becomes as follows:

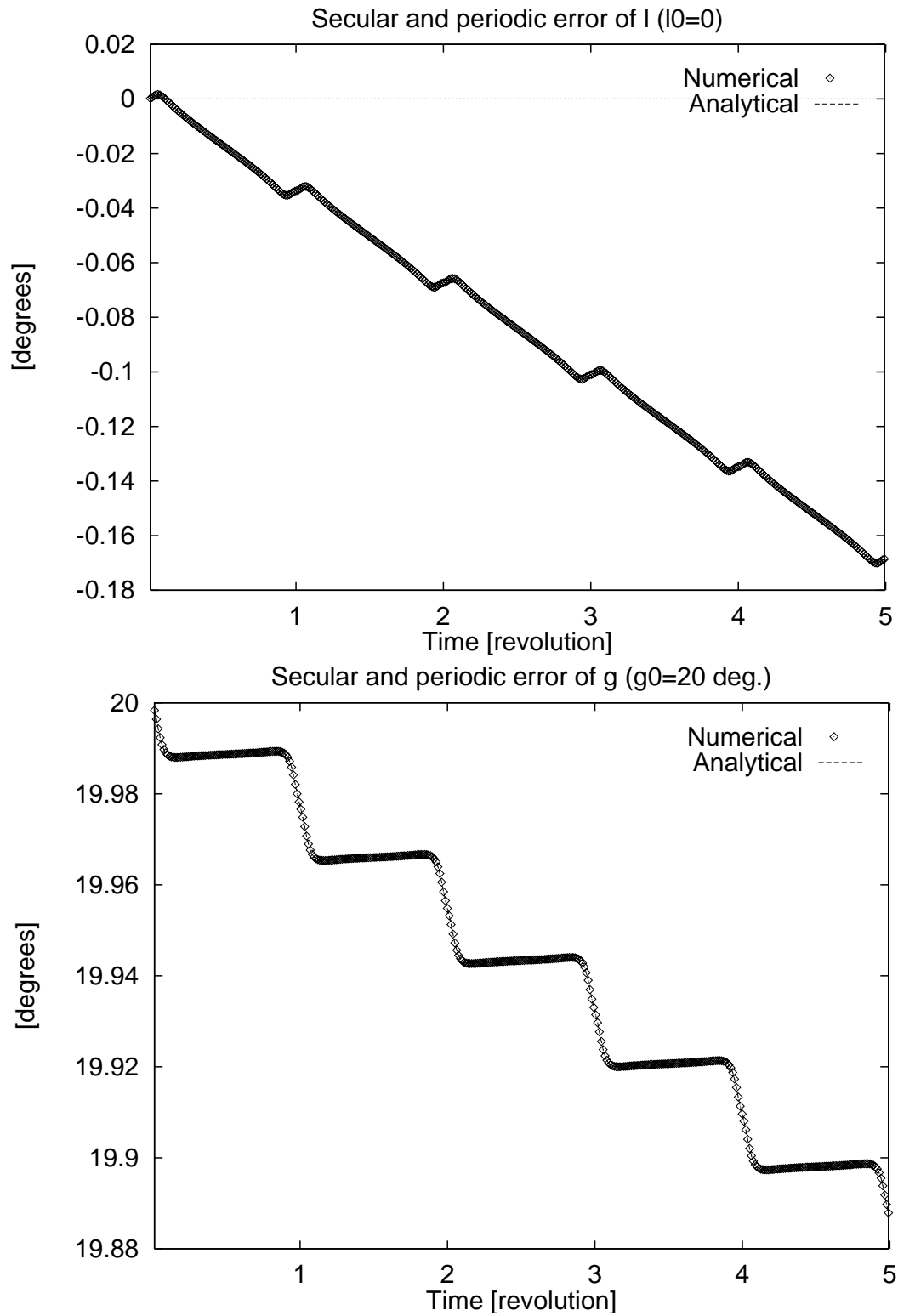
$$\begin{aligned}
l &= l^* + \{l^*, S_1\} \\
&= l^* + \frac{\partial S_1}{\partial L^*} \\
&= l_0 + \frac{\mu^2}{L_0^3} t + \tau^2 n^* \left( -\frac{3a^*}{\mu} H_{1,t=0} + \frac{\mu}{24a^{*3} \eta^{*3}} \right) t \\
&\quad + \frac{\tau^2 \mu^2}{24na^4 \eta^5} \left[ \frac{G^2}{L^3} (f - l) + \frac{G^2}{eL^3} \left\{ \left( 1 - \frac{3e^2}{4} \right) \sin f + \left( e - \frac{e^3}{4} \right) \left( \frac{a}{r} + \frac{L^2}{G^2} \right) \sin f \right. \right. \\
&\quad + \left( 1 + \frac{e^2}{2} \right) \left( \frac{a}{r} + \frac{L^2}{G^2} \right) - \frac{3}{4} \cdot 2e \left( \sin 2f + e \left( \frac{a}{r} + \frac{L^2}{G^2} \right) \cos 2f \right) \\
&\quad \left. \left. - \frac{1}{4} \cdot 3e^2 \left( \sin 3f + e \left( \frac{a}{r} + \frac{L^2}{G^2} \right) \cos 3f \right) \right\} \right]. \tag{107}
\end{aligned}$$

The errors of  $l$  are plotted in upper panels of Figures 3, 4, and 5. The upper panel of Figures 3 shows the secular and periodic errors of  $l$  by the numerical symplectic integration and the analytical perturbation theory, compared with the exact solution of the Keplerian motion. The upper panel of Figures 4 shows only the periodic errors of  $l$ . The upper panel of Figures 5 shows the difference of the periodic errors of  $l$  by the numerical integration and analytical perturbation theory. Higher-order analytical solution will reduce the difference between these two.

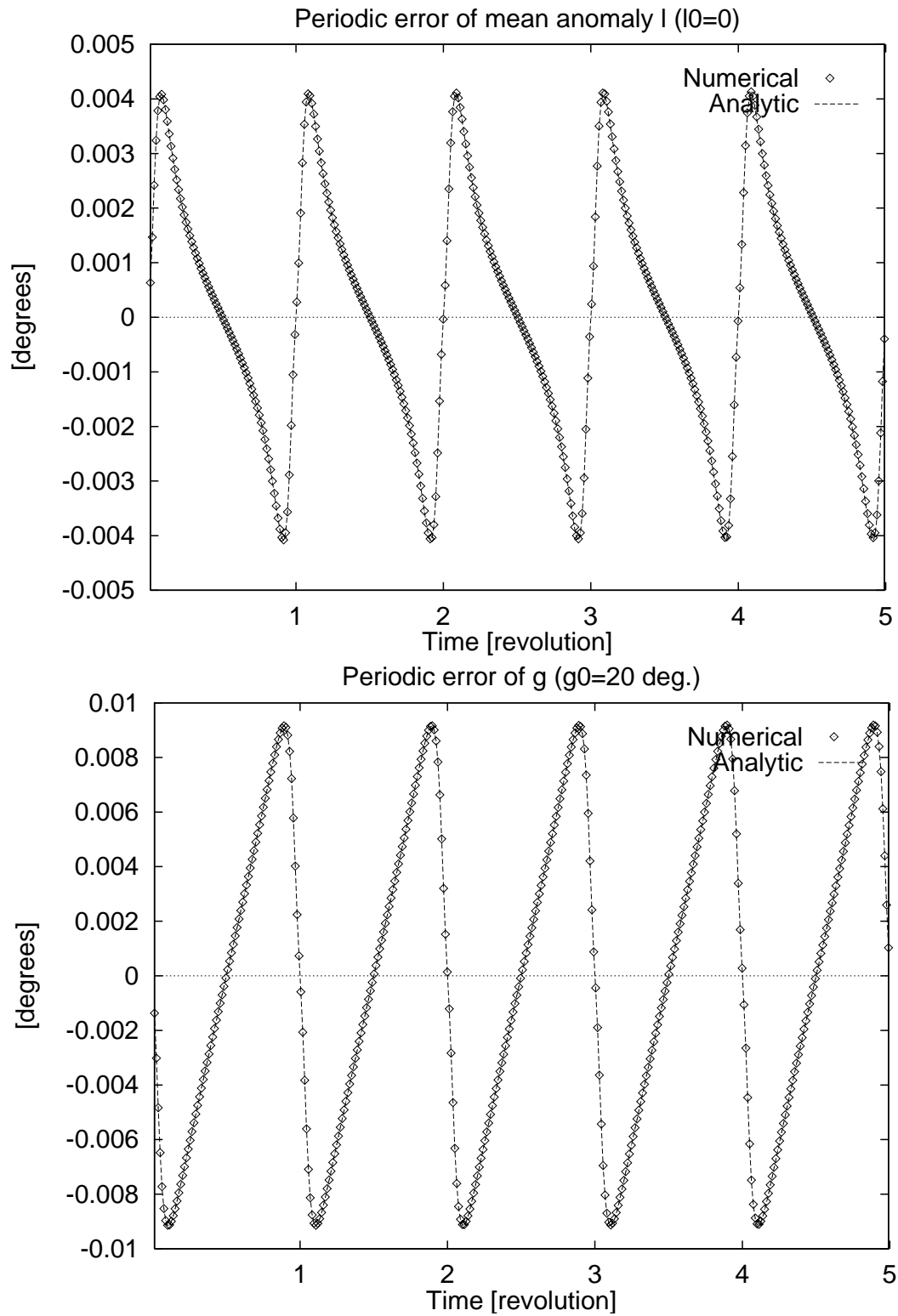
#### 4.5 Solution for $g$

Same as  $l$ ,

$$g = g^* + \{g^*, S_1\}$$



**Figure 3.** The numerical and analytical solution of the secular + periodic errors in  $l$  (upper) and  $g$  (lower), compared with the exact solution of the Keplerian motion. The squares denote the numerical solution by the second-order symplectic integrator, the lines denote the solution by the first-order perturbation theory.



**Figure 4.** The numerical and analytical solution of the periodic errors in  $l$  (upper) and  $g$  (lower), subtracting the secular error shown in Figure 3. The squares denote the numerical solution by the second-order symplectic integrator, the lines denote the solution by the first-order perturbation theory.

$$\begin{aligned}
&= g^* + \left( \frac{\partial g^*}{\partial t^*} \frac{\partial S_1}{\partial L^*} - \frac{\partial g^*}{\partial L^*} \frac{\partial S_1}{\partial t^*} + \frac{\partial g^*}{\partial g^*} \frac{\partial S_1}{\partial G^*} - \frac{\partial g^*}{\partial G^*} \frac{\partial S_1}{\partial g^*} \right) \\
&= g^* + \frac{\partial S_1}{\partial G^*} \\
&= g^* + \frac{\partial}{\partial G^*} \int (H_1 - H_1^*) dt^*. \tag{108}
\end{aligned}$$

Now we know that the secular error of  $g$  is caused from  $g^*$ , and the periodic error of  $g$  is caused from  $\frac{\partial S_1}{\partial G^*}$ .

#### 4.5.1 Secular error of $g$

The canonical equation of motion using  $g^*$  using the new Hamiltonian (75) becomes

$$\begin{aligned}
\frac{dg^*}{dt} &= \frac{\partial H^*}{\partial G^*} \\
&= \frac{\partial}{\partial G^*} \left( -\frac{\mu^2}{L^{*2}} + \frac{\tau^2 \mu^2}{24 a^{*4} \eta^{*5}} \left( 1 + \frac{e^{*2}}{2} \right) \right) \\
&= -\frac{\tau^2 \mu}{4 a^{*3} \eta^{*6}} \left( 1 + \frac{e^{*2}}{4} \right) n. \tag{109}
\end{aligned}$$

$$\therefore g^* = -\frac{\tau^2 \mu}{4 a^{*3} \eta^{*6}} \left( 1 + \frac{e^{*2}}{4} \right) n^* t + g_0. \tag{110}$$

The second term in the right-hand side of (110) represents the the secular error of  $g$  up to the first-order of the perturbation theory.  $g_0$  is the initial value of  $g$  when  $t = 0$ .

#### 4.5.2 Periodic error of $g$

The periodic error of  $g$  can be obtained as the same way as  $l$ . From (108),

$$\begin{aligned}
\frac{dS_1}{dG^*} &= \frac{\partial}{\partial G^*} \int (H_1 - H_1^*) dt^* \\
&= \frac{\partial}{\partial G^*} \int \left[ \frac{\tau^2 \mu^2}{24} \left( \frac{6}{r^{*4}} - \frac{3a^* (1 - e^{*2})}{r^{*5}} - \frac{2}{a^* r^{*3}} \right) - \frac{\tau^2 \mu^2}{24} \frac{1 + \frac{e^{*2}}{2}}{a^{*4} \eta^{*5}} \right] dt^*. \tag{111}
\end{aligned}$$

Same as  $l$ , it is clear that we have to perform the following two calculations successively:

1. Indefinite integration of

$$\int \frac{dt^*}{r^{*n}} = \frac{1}{n^*} \int \frac{dl^*}{r^{*n}}, \quad (n = 3, 4, 5)$$

2. Partial differentiation of the indefinite integrals by  $G^*$ .

The first task has been already done. The second task is given as follows:

$$\begin{aligned}
\frac{\partial S_1}{\partial G^*} &= \frac{\partial}{\partial G^*} \int (H_1 - H_1^*) dt^* \\
&= \frac{\partial}{\partial G^*} \frac{1}{n^*} \int (H_1 - H_1^*) dl^* \\
&= \frac{\partial}{\partial G^*} \left[ \frac{\tau^2 \mu^2}{24 n^* a^{*4} \eta^{*5}} \mathcal{F}(f^*, l^*) \right], \tag{112}
\end{aligned}$$

where  $\mathcal{F}(f^*, l^*)$  denotes the periodic function of  $f^*$  and  $l^*$  described in the integrand of (97) as

$$\mathcal{F}(f^*, l^*) = \left(1 + \frac{e^{*2}}{2}\right) f^* + \left(e^* - \frac{e^{*3}}{4}\right) \sin f^* - \frac{3e^{*2}}{4} \sin 2f^* - \frac{e^{*3}}{4} \sin 3f^* - \left(1 + \frac{e^{*2}}{2}\right) l^*. \quad (113)$$

Henceforward, the variables with superscript  $*$  are replaced by those without  $*$  since all the periodic terms are of the first-order of perturbation. We neglect  $*$  in the following discussion for simplicity.

As for the coefficient part in (112),

$$\frac{\mu^2}{na^4\eta^5} = \frac{a^{\frac{3}{2}}}{\mu^{\frac{1}{2}} a^4\eta^5} \mu^2 = \mu^4 [\mu a (1 - e^2)] = \frac{\mu^4}{G^5}. \quad (114)$$

Therefore

$$\begin{aligned} \frac{\partial S_1}{\partial G} &= \frac{\partial}{\partial G} \int (H_1 - H_1^*) dt^* \\ &= \frac{\tau\mu^4}{24} \left[ \frac{\partial}{\partial G} \left( \frac{\mu}{G^5} \right) \mathcal{F}(f, l) + \frac{1}{G^5} \frac{\partial}{\partial G} \mathcal{F}(f, l) \right]. \end{aligned} \quad (115)$$

It is possible to calculate the partial derivatives of  $\mathcal{F}(f^*, l^*)$  in the same way as in  $l$ :

$$\begin{aligned} \frac{\partial}{\partial G} \left(1 + \frac{e^2}{2}\right) f &= e \frac{\partial e}{\partial G} f + \left(1 + \frac{e^2}{2}\right) \frac{\partial f}{\partial G} \\ &= e \left(-\frac{G}{eL^2}\right) f + \frac{\partial e}{\partial G} \left(1 + \frac{e^2}{2}\right) \left(\frac{a}{r} + \frac{L^2}{G^2}\right) \sin f, \end{aligned} \quad (116)$$

$$\frac{\partial}{\partial G} \left(1 + \frac{e^2}{2}\right) l = e \frac{\partial e}{\partial G} l = e \left(-\frac{G}{eL^2}\right) l, \quad (117)$$

$$\begin{aligned} \frac{\partial}{\partial G} \left(e - \frac{e^3}{4}\right) \sin f &= \left(1 - \frac{3e^2}{4}\right) \frac{\partial e}{\partial G} \sin f + \left(e - \frac{e^3}{4}\right) \cos f \frac{\partial f}{\partial G} \\ &= \frac{\partial e}{\partial G} \left[ \left(e - \frac{3e^2}{4}\right) \sin f + \left(e - \frac{e^3}{4}\right) \cos f \left(\frac{a}{r} + \frac{L^2}{G^2}\right) \sin f \right], \end{aligned} \quad (118)$$

$$\begin{aligned} \frac{\partial}{\partial G} (e^2 \sin 2f) &= 2e \frac{\partial e}{\partial G} \sin 2f + 2e^2 \cos 2f \frac{\partial f}{\partial G} \\ &= \frac{\partial e}{\partial G} \left[ 2e \sin 2f + 2e^2 \cos 2f \left(\frac{a}{r} + \frac{L^2}{G^2}\right) \sin f \right], \end{aligned} \quad (119)$$

$$\begin{aligned} \frac{\partial}{\partial G} (e^3 \sin 3f) &= 3e^2 \frac{\partial e}{\partial G} \sin 3f + 3e^3 \cos 3f \frac{\partial f}{\partial G} \\ &= \frac{\partial e}{\partial G} \left[ 3e^2 \sin 3f + 3e^3 \cos 3f \left(\frac{a}{r} + \frac{L^2}{G^2}\right) \sin f \right]. \end{aligned} \quad (120)$$



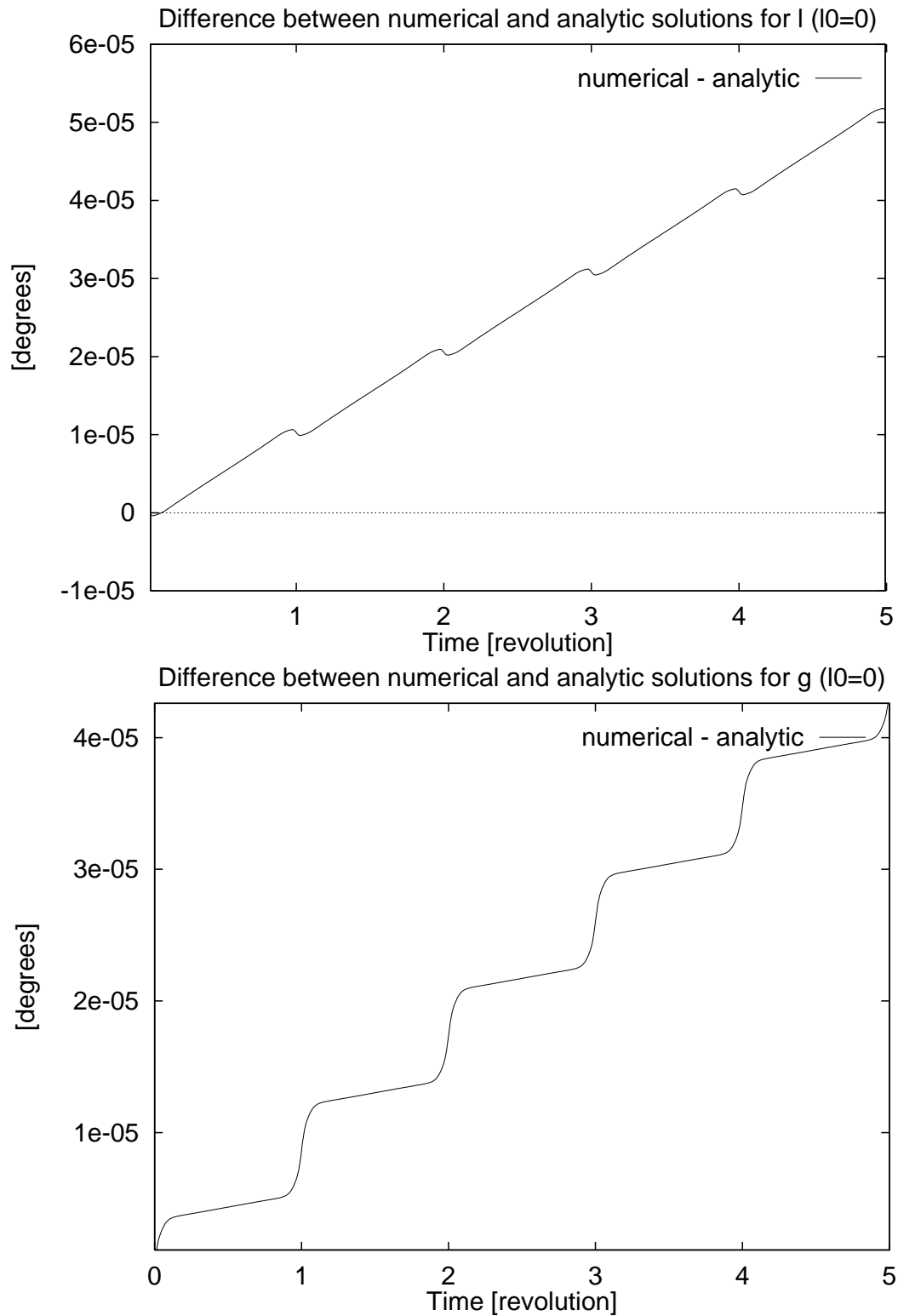
Substituting (116)(117)(118)(119)(120) into (112), periodic errors of  $g$  becomes

$$\begin{aligned}
\frac{\partial S_1}{\partial G^*} &= \frac{\partial}{\partial G^*} \int (H_1 - H_1^*) dt^* \\
&= \frac{\tau^2 \mu^4}{24} \left[ -\frac{5}{G^6} \left\{ \left(1 + \frac{e^2}{2}\right) (f - l) + \left(e - \frac{e^3}{4}\right) \sin f - \frac{3e^2}{4} \sin 2f - \frac{e^3}{4} \sin f \right\} \right. \\
&\quad + \frac{1}{G^5} \left\{ -\frac{G}{L^2} (f - l) - \frac{G}{eL^2} \left( \left(1 + \frac{e^2}{2}\right) \left(\frac{a}{r} + \frac{L^2}{G^2}\right) \right. \right. \\
&\quad \quad \left. \left. + \left(1 - \frac{3e^2}{4}\right) \sin f + \left(e - \frac{e^3}{4}\right) \cos f \left(\frac{a}{r} + \frac{L^2}{G^2}\right) \right. \right. \\
&\quad \quad \left. \left. - \frac{3}{2} e \left( \sin 2f + e \cos 2f \left(\frac{a}{r} + \frac{L^2}{G^2}\right) \right) \right. \right. \\
&\quad \quad \left. \left. - \frac{3}{4} e^2 \left( \sin 3f + e \cos 3f \left(\frac{a}{r} + \frac{L^2}{G^2}\right) \right) \right) \right\} \right]. \tag{121}
\end{aligned}$$

Therefore, from (108) and (121), final solution for  $g$  up to the first-order perturbation can be obtained as follows:

$$\begin{aligned}
g &= g^* + \{g^*, S_1\} \\
&= g^* + \frac{\partial S_1}{\partial G^*} \\
&= g_0 - \frac{\tau^2 \mu}{4a^{*3} \eta^{*6}} \left(1 + \frac{e^{*2}}{4}\right) n^* t \\
&\quad + \frac{\tau^2 \mu^4}{24} \left[ -\frac{5}{G^6} \left\{ \left(1 + \frac{e^2}{2}\right) (f - l) + \left(e - \frac{e^3}{4}\right) \sin f - \frac{3e^2}{4} \sin 2f - \frac{e^3}{4} \sin f \right\} \right. \\
&\quad \quad + \frac{1}{G^5} \left\{ -\frac{G}{L^2} (f - l) - \frac{G}{eL^2} \left( \left(1 + \frac{e^2}{2}\right) \left(\frac{a}{r} + \frac{L^2}{G^2}\right) \right. \right. \\
&\quad \quad \quad \left. \left. + \left(1 - \frac{3e^2}{4}\right) \sin f + \left(e - \frac{e^3}{4}\right) \cos f \left(\frac{a}{r} + \frac{L^2}{G^2}\right) \right. \right. \\
&\quad \quad \quad \left. \left. - \frac{3}{2} e \left( \sin 2f + e \cos 2f \left(\frac{a}{r} + \frac{L^2}{G^2}\right) \right) \right. \right. \\
&\quad \quad \quad \left. \left. - \frac{3}{4} e^2 \left( \sin 3f + e \cos 3f \left(\frac{a}{r} + \frac{L^2}{G^2}\right) \right) \right) \right\} \right]. \tag{122}
\end{aligned}$$

The solution for  $g$  is plotted in the lower panels of Figures 3, 4, and 5. The lower panel of Figures 3 shows the secular and periodic errors of  $g$  by the numerical symplectic integration and analytical perturbation theory, compared with the exact solution of the Keplerian motion. The lower panel of Figures 4 shows only the periodic errors of  $g$ . The lower panel of Figures 5 shows the difference of the periodic errors of  $g$  by the numerical integration and the analytical perturbation theory. Higher-order analytical solution will reduce the difference between these two.



**Figure 5.** The differences of the periodic errors of  $l$  (upper) and  $g$  (lower) obtained by the numerical and analytical methods, which are equivalent to the differences in two data (squares and lines) in Figure 3.

## 4.6 Another interpretation of the numerical error source

The principle source of the numerical error by symplectic integration is that of mean anomaly  $l$ , which grows linearly in time. According to Kinoshita et al. (1991), we can derive the source of the secular numerical error of  $l$  (89) as follows: The mean anomaly  $\tilde{l}$  of the surrogate system is dominated by the surrogate Hamiltonian  $\tilde{H}$ , and the mean anomaly  $l$  of the real system is dominated by the real Hamiltonian  $H$ . The equations of motion which  $\tilde{l}$  and  $l$  follow except for periodic parts would be

$$\frac{d\tilde{l}}{dt} = \frac{\partial \tilde{H}}{\partial L}, \quad (123)$$

$$\frac{dl}{dt} = \frac{\partial H}{\partial L}, \quad (124)$$

respectively. Subtracting (124) from (123), we get

$$\begin{aligned} \frac{d}{dt} (\tilde{l} - l) &= \frac{\partial \tilde{H}}{\partial L} - \frac{\partial H}{\partial L} \\ &= \frac{\partial H_{\text{err}}}{\partial L} \\ &= -\frac{\tau^2 \mu n}{12a^3 \eta^5} \left( 1 + \frac{5e^2}{4} \right), \end{aligned} \quad (125)$$

which is equal to Eq. (19) in Kinoshita et al. (1991), and also coincides with the second term of the right-hand side of our (86) except for the superscript  $*$ .

In addition to (125), there is another source of the secular truncation error in the mean anomaly  $l$  due to the constant part of the truncation error the total energy,  $E$ . Since the surrogate Hamiltonian  $\tilde{H}$  is strictly preserved by symplectic integration, we have

$$\tilde{H} = H(\mathbf{q}_0, \mathbf{p}_0) + H_{\text{err}}(\mathbf{q}_0, \mathbf{p}_0) = H(\mathbf{q}, \mathbf{p}) + H_{\text{err}}(\mathbf{q}, \mathbf{p}), \quad (126)$$

to  $O(\tau^2)$  approximation.  $(\mathbf{q}_0, \mathbf{p}_0)$  are initial values, and  $(\mathbf{q}, \mathbf{p})$  are the approximate solutions obtained by the symplectic integration. From (126), the truncation error of the total energy (i.e. secular part of Hamiltonian) becomes

$$\Delta E = H(\mathbf{q}, \mathbf{p}) - H(\mathbf{q}_0, \mathbf{p}_0) = H_{\text{err}}(\mathbf{q}_0, \mathbf{p}_0) - H_{\text{err}}(\mathbf{q}, \mathbf{p}). \quad (127)$$

Since  $H_{\text{err}}(\mathbf{q}_0, \mathbf{p}_0)$  is fixed, constant part of  $\Delta E$  is given by

$$\begin{aligned} \Delta E_c \equiv \langle \Delta E \rangle &= \langle H_{\text{err}}(\mathbf{q}_0, \mathbf{p}_0) - H_{\text{err}}(\mathbf{q}, \mathbf{p}) \rangle \\ &= H_{\text{err}}(\mathbf{q}_0, \mathbf{p}_0) - \langle H_{\text{err}}(\mathbf{q}, \mathbf{p}) \rangle \\ &= H_{\text{err}}(\mathbf{q}_0, \mathbf{p}_0) - \frac{\tau^2 \mu^2}{24a^4 \eta^5} \left( 1 + \frac{e^2}{2} \right). \end{aligned} \quad (128)$$

In general, we can derive the constant bias in semimajor axis ( $\Delta a$ ) due to the constant part of orbital energy offset ( $\Delta E_c$ ) as follows:

$$E = -\frac{\mu}{2a}, \quad (129)$$

$$\therefore a = -\frac{\mu}{2E}, \quad (130)$$

$$\therefore \Delta a = \frac{\mu}{2E^2} \Delta E_c. \quad (131)$$

Hereafter we use  $\Delta E_c$  instead of  $\Delta E$  in order to remark explicitly it is constant.

From the Kepler's third law,  $n^2 a^3 = \mu$  is fixed in the gravitational two-body problem. Then the secular error of  $l$  due to  $\Delta a$  can be obtained by taking a variation of the Kepler's third law:

$$2\Delta n \cdot a^3 + n^2 \cdot 3a\Delta a = 0, \quad (132)$$

$$\therefore 2\Delta n a + 3n\Delta a = 0. \quad (133)$$

If we are to express the variation of the time derivative of  $l$  as

$$\frac{d}{dt} (\tilde{l} - l) = \Delta \dot{l} = \Delta n, \quad (134)$$

the secular error of  $l$  becomes from (133)

$$\Delta \dot{l} = \Delta n = -\frac{3n\Delta a}{2a}. \quad (135)$$

Hence the additional secular truncation error of the mean anomaly  $l$  due to  $\Delta E_c$  is from (128) and (131)

$$\begin{aligned} \Delta \dot{l} &= -\frac{3n\Delta a}{2a} \\ &= -\frac{3n}{2a} \cdot \frac{\mu}{2E^2} \cdot \Delta E_c \\ &= -\frac{3n\mu}{4a} \left(-\frac{2a}{\mu}\right)^2 \left[ H_{\text{err}}(\mathbf{q}_0, \mathbf{p}_0) - \frac{\tau^2 \mu^2}{24a^4 \eta^5} \left(1 + \frac{e^2}{2}\right) \right] \\ &= -\frac{3an}{\mu} H_{\text{err}}(\mathbf{q}_0, \mathbf{p}_0) + \frac{\tau^2 \mu n}{8a^3 \eta^5} \left(1 + \frac{e^2}{2}\right). \end{aligned} \quad (136)$$

Now we have the total secular truncation errors for the mean anomaly  $l$  by adding (125) and (136) as

$$\begin{aligned} \Delta \dot{l} &= -\frac{\tau^2 \mu n}{12a^3 \eta^5} \left(1 + \frac{5e^2}{4}\right) + \left[ -\frac{3an}{\mu} H_{\text{err}}(\mathbf{q}_0, \mathbf{p}_0) + \frac{\tau^2 \mu n}{8a^3 \eta^5} \left(1 + \frac{e^2}{2}\right) \right] \\ &= -\frac{3an}{\mu} H_{\text{err}}(\mathbf{q}_0, \mathbf{p}_0) + \frac{\tau^2 \mu n}{24a^3 \eta^5}, \end{aligned} \quad (137)$$

which is equal to the second term of the right-hand side of our (89).

However, this derivation in Kinoshita et al. (1991) is somewhat confusing in spite of its correct solution in (137). Especially, the appearance of the second source of the secular error  $\Delta \dot{l}$  (136) seems to be too abrupt. This is caused by the confusion of  $L$  and  $L^*$  in (125). After the operation of time-averaging (by a certain canonical transformation),  $L^*$ , instead of  $L$ , must be used to describe the canonical equation of motion; (125) should be derived correctly from the canonically transformed equations of motion such as

$$\frac{dl^*}{dt} = -\frac{\partial H^*}{\partial L^*}. \quad (138)$$

Moreover, the averaged value of  $L$  is not equal to  $L^*$ ;  $L^*$  has a constant bias to  $L$ , which is the true reason of the “another source of the secular truncation error in the mean anomaly due to the constant part of the truncation error in the energy” in Kinoshita et al. (1991). The detailed and exact form of  $L^*$  is presented in (80) in the previous sections.

#### 4.7 Dependence on initial configuration

As you can see in the equation (107), the secular numerical error in  $l$  arises from the coefficient of  $t$ , namely

$$\delta n_{\text{sec}} \equiv \tau^2 n \left( -\frac{3a}{\mu} H_{1,t=0} + \frac{\mu}{24a^3 \eta^3} \right). \quad (139)$$

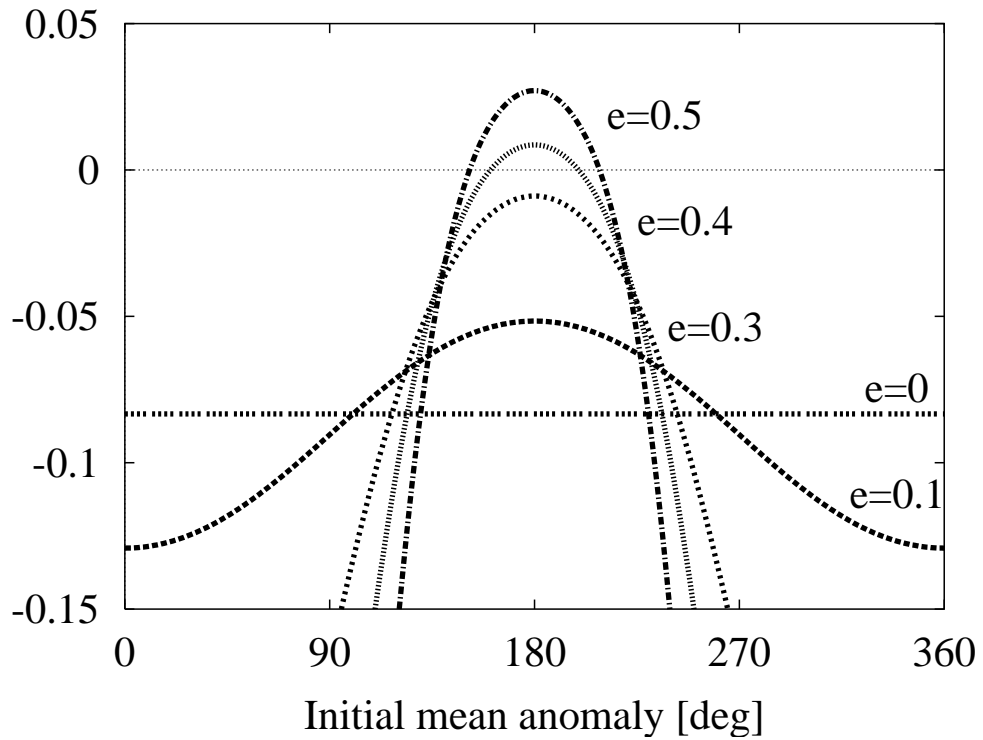
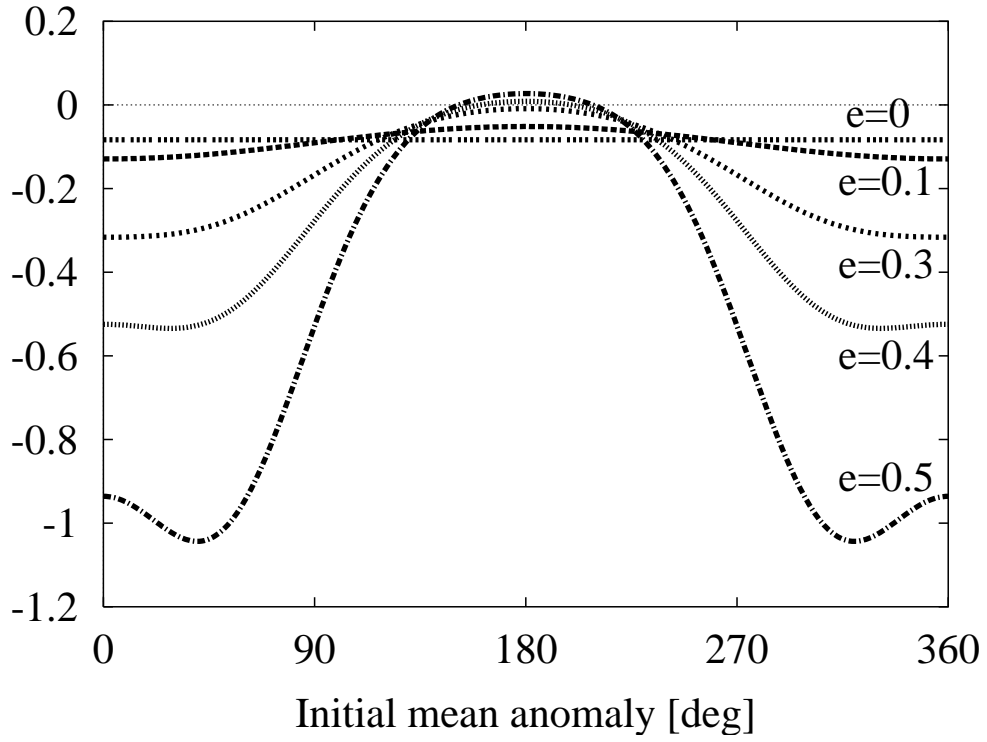
Hereafter we call the coefficient (139)  $\delta n_{\text{sec}}$ . Note that in the expression of  $\delta n_{\text{sec}}$  in (139) we neglected all of the superscripts  $*$ .

Not only  $\delta n_{\text{sec}}$  has a dependence on the initial longitude in  $H_{1,t=0}$  as discussed in the previous sections, but this has a dependence on the initial orbital shape,  $e$ . The effect of  $a$  is only to scale the unit of time, so we can neglect it from the discussion of numerical error here. We plot this  $\delta n_{\text{sec}}$ 's dependence on initial eccentricity as well as initial starting longitude in the two-body problem in Figure 6. We can anticipate from (139) that there are certain initial mean anomalies ( $l_0$ ) which make  $\delta n_{\text{sec}}$  very small, possible zero. Actually in some cases of higher eccentricities,  $\delta n_{\text{sec}}$  becomes zero at certain values of initial mean anomaly in Figure 6. However, generally  $\delta n_{\text{sec}}$  does not become zero whatever we change the initial mean anomaly.

In Figure 7, we exaggeratedly illustrate the trajectories of  $(l, L)$  of the two-body system described in this section. “Exact” denotes the exact solution which goes from  $(1, 0)$  and comes back at  $(1, 0)$  again. “Numerical” denotes the symplectic numerical solution which goes from a different point from  $(1, 0)$  and does not come back at the starting point. “Synthetic” denotes the analytical secular solution obtained by the perturbation theory which is close to the time-average of the numerical solution. As we see, the exact and the synthetic solutions are far from coincidence when the initial mean anomaly  $l_0 = 0$  (left panel), while they coincide pretty well when the initial mean anomaly  $l_0 = 180^\circ$  (right panel). This result corresponds to the result shown in Figure 6 in terms of the numerical error of the symplectic integrator.

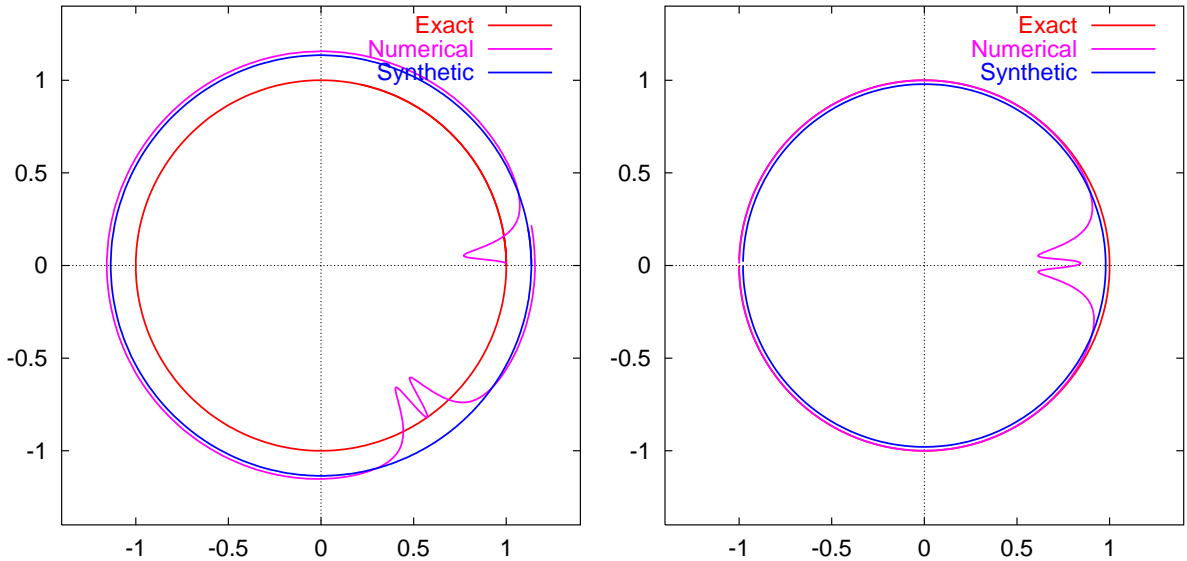
### 5. Reduction of errors by the iterative start

In the examples of Kepler problem in the previous sections, we could find an approximate analytical solution of symplectic numerical error by a perturbation theory. However in general many-body systems, it is quite difficult, or virtually impossible, to obtain an analytical form of the numerical error; hence we cannot know which initial mean anomaly would reduce the numerical error of symplectic integrator in analytical way. Thus we have to depend on a numerical way to look for the initial conditions which reduce numerical errors. This kind of numerical method we use when we start our integration has been originally proposed by Saha & Tremaine (1992) under the name of “iterative start.” Our method is essentially the same with their iterative start, but a bit different in its way of implementation. We mention our method and results in two kinds of three-body dynamical system: Sun–Jupiter and a fictitious



**Figure 6.** (Upper) the secular error coefficient of mean anomaly in the two-body problem (139) as a function of initial mean anomaly  $l_0$ . Five curves show the results when  $e = 0, 0.1, 0.3, 0.4,$  and  $0.5$ . (Lower) an enlarged panel of the central part of the upper one.

middle-sized body in the asteroidal belt, and a planet orbiting around a binary system named MACHO-97-BLG-41 which has been discovered by a gravitational microlensing event.



**Figure 7.** Exaggerated illustration of the trajectories of  $(l, L)$  of the two-body system (see Table 1). (Left) when  $l_0 = 0$ . (Right) when  $l_0 = 180^\circ$ . The line denoted “Exact” shows the exact solution which goes from  $(1, 0)$  and comes back at  $(1, 0)$  again. The line “Numerical” denotes the symplectic numerical solution which goes from a different point from  $(1, 0)$  and does not come back at the starting point. The line “Synthetic” means the analytical secular solution obtained by the perturbation theory which is close to the time-average of the numerical solution. We have intentionally exaggerated the deviation of the numerical and synthetic solutions from the exact ones in order to bring out the difference.

## 5.1 Perturbed motion of a middle-sized planet

### 5.1.1 Settings of numerical experiments

First we consider a weakly perturbed three-body system, Sun–Jupiter and a fictitious middle-sized body in the asteroidal belt (see Figure 8). The fictitious middle-sized body has a finite mass of  $1/10 M_{\text{Jupiter}}$ , hence the problem is not a restricted one. The initial orbital elements of the middle-sized body are similar to those of Ceres: when  $e = 0.1$  and  $e = 0.4$ ,  $a = 2.6\text{AU}$ . When  $e = 0.6$ ,  $a = 2.2\text{AU}$  so that we avoid its close encounters with the outer planet. The values of other orbital elements than  $a$  or  $e$  are the same as those of Ceres. The mass and initial orbital elements of the outer massive planet in this system is just the same as those of Jupiter. These initial orbital elements of the bodies are basically taken from the Development Ephemeris of JPL, DE245 (Standish, 1990).

A principle way to execute the “iterative start” in this section is as follows:

1. Given a nominal set of initial orbital elements, perform an integration with a very high

accuracy covering a shorter timespan than the main integration.

2. Choose several initial conditions of all relevant bodies from the results of the accurate integration.
3. Perform several short-term integrations with a normal accuracy using the initial conditions selected above.
4. Calculate the numerical differences between the accurate integration and each of the short-term integration.
5. Select an initial condition which produces the least numerical error as the set of starting orbital elements of the main integration.
6. Perform the main integration using the initial condition selected above.

Note that the integration periods of the accurate integration and the short-term integrations are much shorter than the period of the main integration. For example, when the period of the main integration is  $1 \times 10^8$  years, we would take a  $10^4$ -year for the accurate and the short-term integration periods. The initial conditions for the short-term integrations are chosen while the Jupiter-like planet orbits the Sun once (about twelve years). Interval among each initial condition is  $\sim 1^\circ$  in the Jupiter-like planet's longitude, or about ten days in time. We have illustrated the situation in Figure 9.

When perturbation to the Kepler motion is very small, we may be able to implement the “iterative start” on the system in a simpler way as follows:

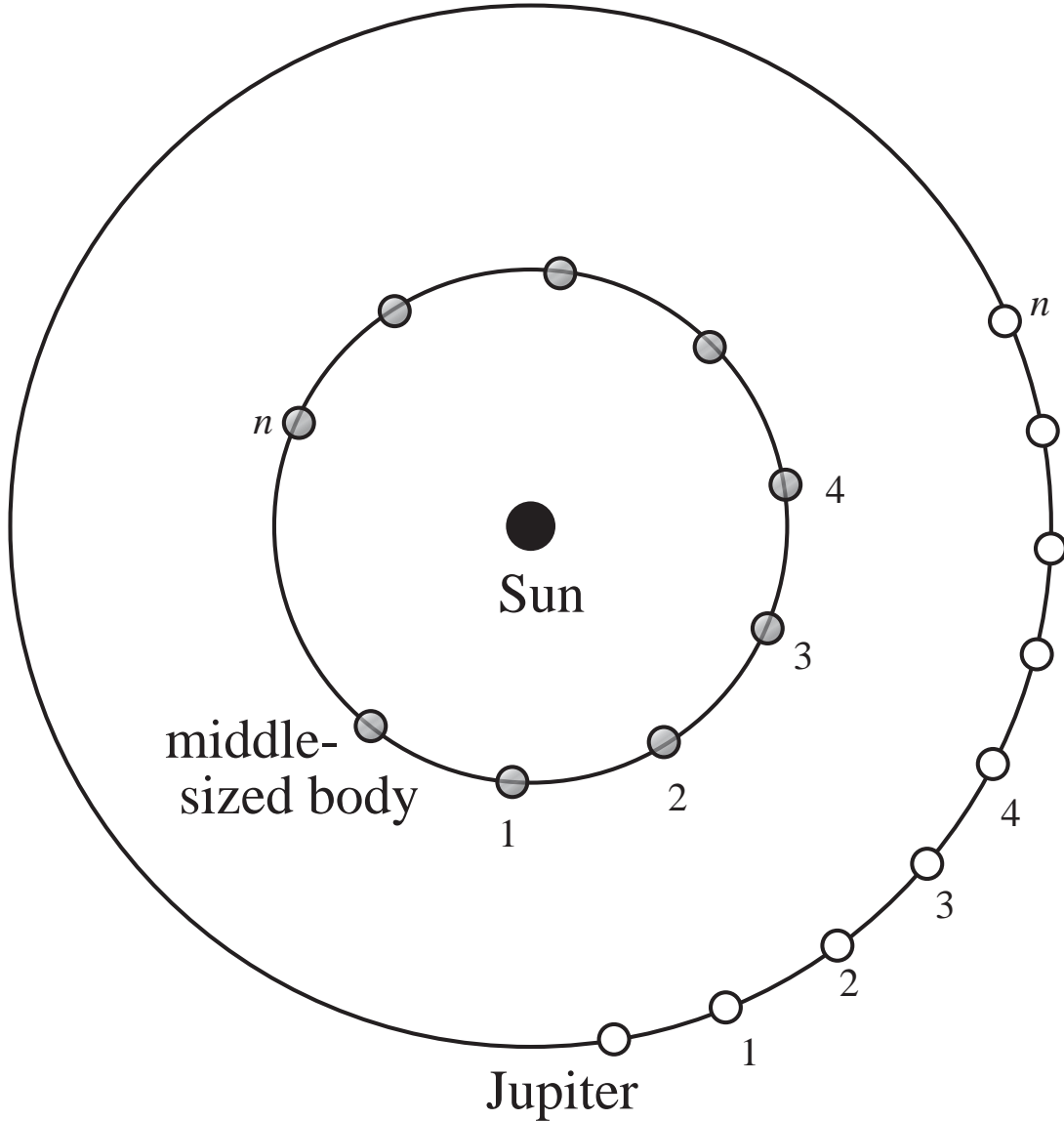
1. Given a nominal set of initial orbital elements, we can fix the Keplerian osculating orbital orbits of each body.
2. Let each body move on its osculating orbit by a small interval (see Figure 8).
3. Name each position as  $1, 2, 3, \dots, n$ . At each position, perform two sets of numerical integrations of a short period: one is a very accurate integration, and the other's accuracy is the same as that of the main integration.
4. Compare the two sets of integrations and calculate their numerical difference at each position from 1 to  $n$ .
5. Repeat the above comparison until we reach a certain point,  $n$ .
6. Select an initial condition which produces the least numerical difference as the starting orbital elements of the main integration.
7. Perform the main integration using the set of initial condition selected above.

In the discussions below, we choose the latter procedure. Note again that the procedure is valid only for a slightly disturbed system such as the Sun–Jupiter–a middle-sized planet. We cannot apply this simplified procedure to a significantly perturbed system like the planetary



system around a binary which we will discuss later. This is due to a stronger perturbation on the planetary orbit from the short-term orbital motion of binary.

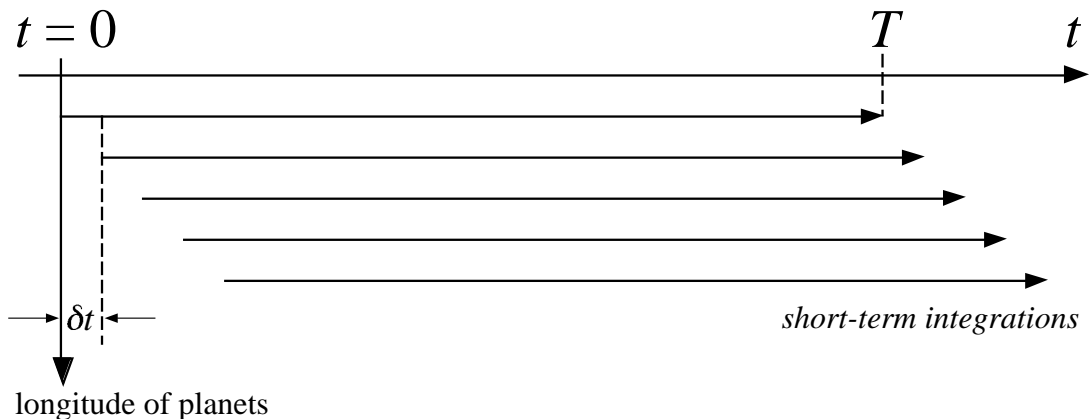
We fix the period of the accurate and the short-term integrations as  $2 \times 10^4$  years. We take the time interval of each set of initial condition as  $P_{\text{Jupiter}}/360$  where  $P_{\text{Jupiter}}$  is the orbital period of Jupiter. We choose 360 sets of initial conditions for comparison, meanwhile Jupiter rotates around the Sun once, and the middle-sized planet does twice or more.



**Figure 8.** A schematic illustration of the Sun–Jupiter–a middle-sized body system. Each short-term integration starts at the numbered position from  $1, \dots, n$ . See also Figure 9.

### 5.1.2 Results of the numerical experiments

We have performed numerical experiments for the three-body planetary system using the second-order explicit symplectic integrator described in Section 3.. As for canonical variables



**Figure 9.** A schematic illustration of our way of implementation of the “iterative start.” Each short-term integration starts at a different time (or a different orbital position) on a same dynamical trajectory. See also Figure 8.

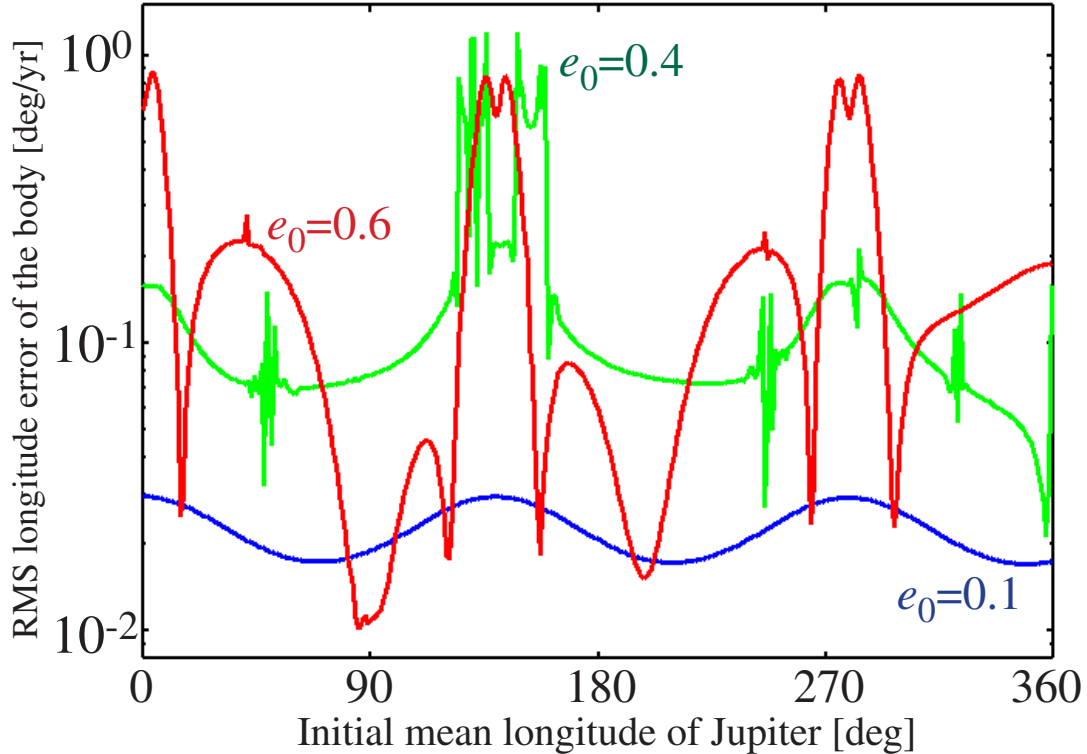
used in the scheme, we have adopted the Jacobi coordinate. The shorter integrations are done with a stepsize of 4 days. As the standard numerical integration with a high accuracy, we have performed an integration over  $2 \times 10^4$ -year period with a stepsize of  $0.0625 = 1/16$  days. We consider this standard integration much more accurate than the shorter integrations, and calculate the longitudinal difference of the middle-sized planet between the standard integration and the shorter integrations. We have chosen 360 sets of initial orbital conditions while Jupiter revolves once around the Sun from its initial position. We have tested three sets of numerical integrations, changing initial eccentricity of the middle-sized planet  $e_0$ ;  $e_0 = 0.1, 0.4$ , and  $0.6$ . For  $e_0 = 0.6$  set, the initial semimajor axis of the middle-sized planet is set as  $a_0 = 2.2\text{AU}$  so that we avoid its close encounter with Jupiter. In other sets,  $a_0 = 2.2\text{AU}$  which is similar to the semimajor axis of Ceres.

The root-mean-square (RMS) of the longitudinal error of the middle-sized planet per year is shown in Figure 10. Here the horizontal axis is denoted as the initial mean longitude of Jupiter, but note that the initial mean longitude of the middle-sized planet changes accordingly. If we fix the mean longitude of one planet and change that of another, it ends up with integration of the orbital motion in many different dynamical systems. This is not what we mean to study in this manuscript.

In Figure 10, we notice three interesting characters. First, root mean square (RMS) of the longitudinal error of the middle-sized planet differs a lot, depending on initial starting point on the dynamical system. Second, the rate of error reduction is much larger when the initial eccentricity of the middle-sized planet ( $e_0$ ) is large. When  $e_0 = 0.6$ , maximum difference of the RMS is nearly two orders of magnitude. Third, there are some spike-like features on the RMS curves, especially when  $e_0 = 0.4$ .

As for the first point, we can understand it in analogy with the similar analysis in the two-body problem discussed before. Since in Figure 10 there is no zero-axis in ordinate because the figure draws the RMS of the planet’s longitudinal error, we drawn a simple average of the longitudinal error when  $e_0 = 0.6$  in Figure 11. We clearly see that under certain values of

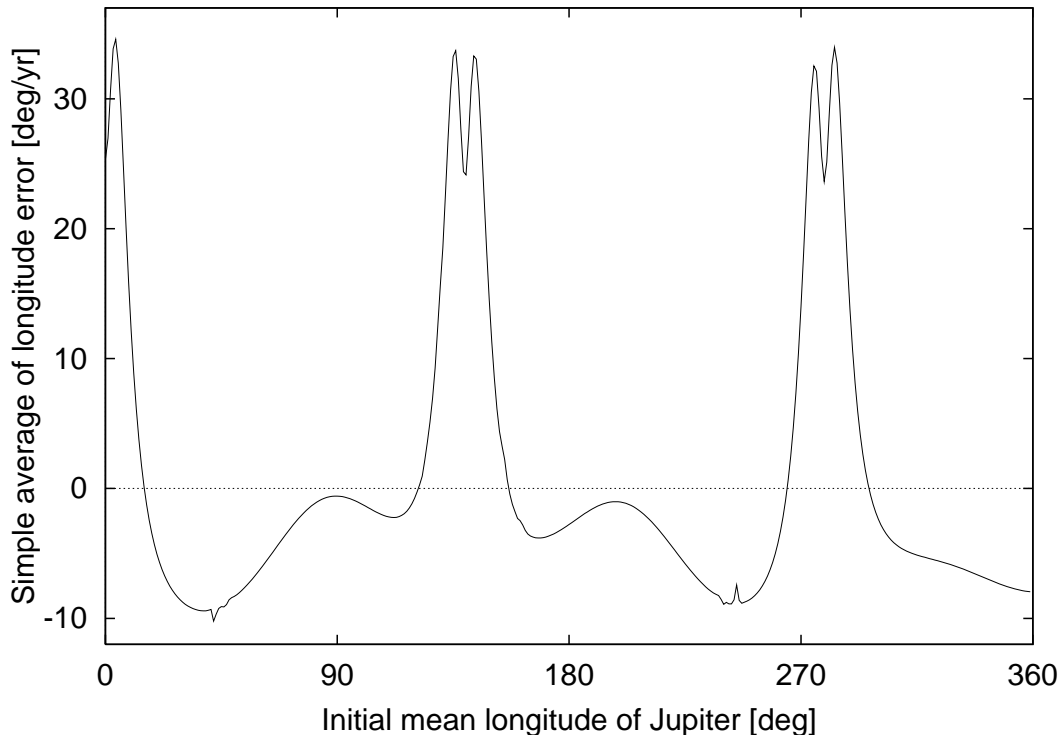
the initial conditions, the longitudinal error crosses zero axis. This means when we start the integrations from such initial conditions that lies on the zero-axis in Figure 11, we can reduce the longitudinal error of the planet to a large extent. In contrast when we choose a bad initial condition, the longitudinal error of the planet increases terribly, which degrades the accuracy of numerical integration very much.



**Figure 10.** The RMS numerical error of the middle-sized planet (deg/year) as a function of Jupiter’s initial mean longitude.  $e_0$  is the initial eccentricity of the the middle-sized planet.

As for the second point, we see the same trend as in the two-body problem discussed below (see Figure 6). We chose some of the typical numerical results of time-series and showed them in Figures 12 ( $e_0 = 0.1$ ), 13 ( $e_0 = 0.4$ ), and 14 ( $e_0 = 0.6$ ). When the initial eccentricity of the middle-sized planet is not so large as  $e_0 = 0.1$ , the degrees of the error reduction by the iterative start is not prominent. However as  $e_0$  grows, the degree of the error reduction becomes larger, even up to two orders of magnitude (the lower panel in Figure 14). We could find five initial conditions where the longitudinal error of the middle-sized planet becomes very small (or possible zero) when  $e_0 = 0.6$  as in Figure 11. But there is only one condition when  $e_0 = 0.4$  (near  $l_{J0} = 360^\circ$ ). When  $e_0 = 0.1$ , we could not find any of such appropriate initial conditions.

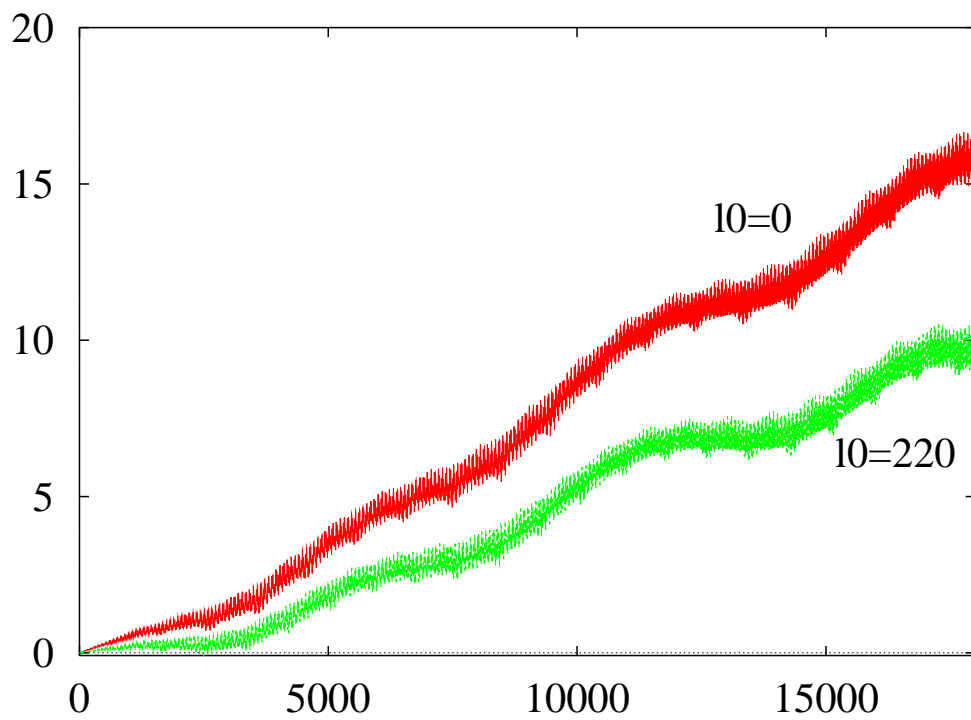
At present we do not have a definite answer why these numerical errors can be significantly reduced much when the initial eccentricity is low in the two-body and weakly perturbed three-body systems such as discussed above. It may be related to a kind of geometry in phase-space of the dynamical system. A simple guess goes on like this: when the eccentricities of bodies are large, geometry of the trajectory in phase-space is somewhat distorted or warped. This distortion could be common in both the real system dominated by Hamiltonian  $H$  and the



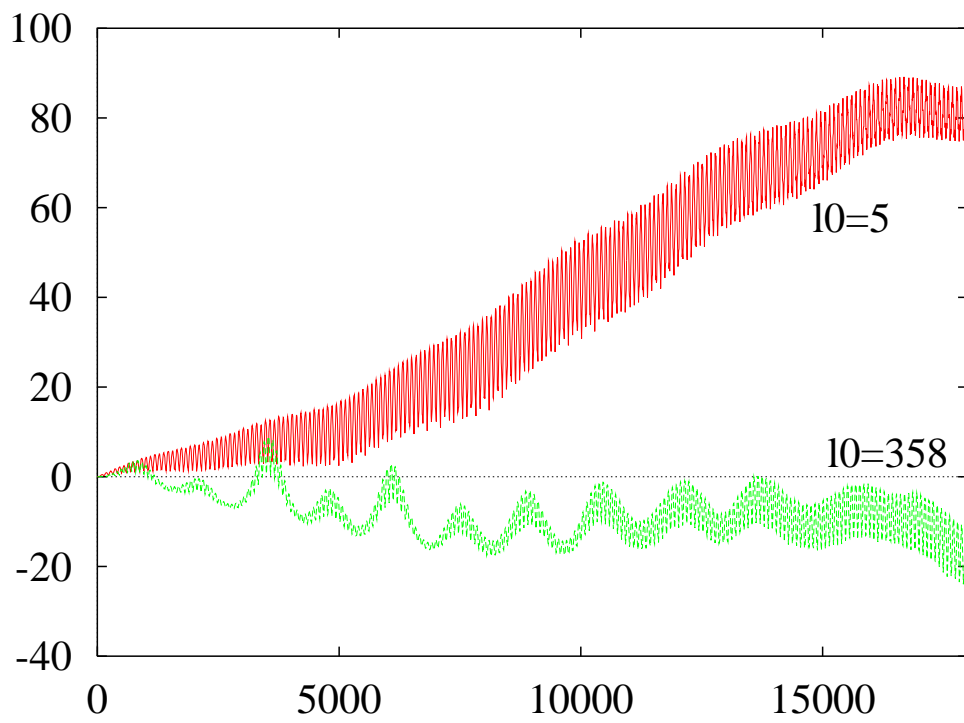
**Figure 11.** The averaged (simple sum) numerical error of the middle-sized planet (deg/year) as a function of Jupiter’s initial mean longitude when  $e_0 = 0.6$  in Figure 10.

surrogate system dominated by surrogate Hamiltonian  $\tilde{H}$  in (21). The initial conditions by which we can significantly reduce numerical error may be intersection points (possibly lines or plains if dimension of the phase-space is large) of the two distorted trajectories. On the other hand when the initial eccentricities of the bodies are small, the trajectory may be very smooth, and the possibility that the two trajectories intersect with each other may become lower, which leads to the non-existence of the initial conditions that reduce the longitudinal error to nearly zero in our numerical experiments. This discussion is still a simple guess. We have to seek a definitive answer confirming the structure of the phase-space in detail.

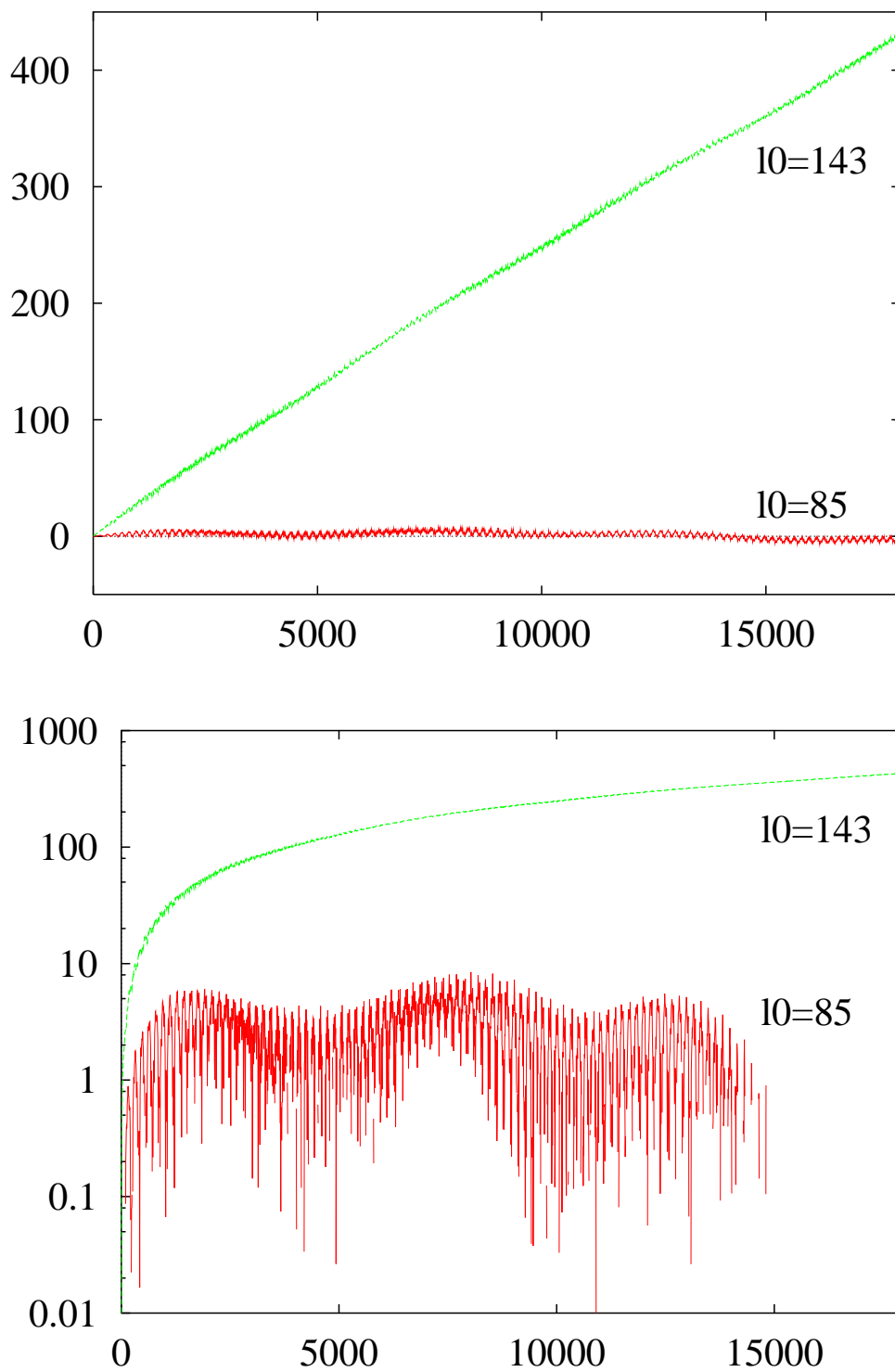
As for the reason of the third point of the spike-like feature, it is not obvious to explain. We took an example result of such spike-like features and showed what was going on there (Figure 15). The figure can be a counterpart of Figure 13 which shows an example time-series when  $e_0 = 0.4$  with  $l_{J0} = 358^\circ$  and  $l_{j0} = 5^\circ$ . When  $l_{J0} = 148^\circ$  that is just on the spike-like area, at the beginning the longitudinal error increases similarly to the results when  $l_{j0} = 5^\circ$ . However when when  $t > 5000$  years, the slope of the curve of  $l_{J0} = 148^\circ$  suddenly increases, and the error increases rapidly afterwards. This nonlinear behavior of the numerical error may be similar to the stepsize resonance phenomena reported in WH-type symplectic integrator (Wisdom and Holman, 1992; Rauch and Holman, 1999) or symmetric multistep methods (Quinlan and Tremaine, 1990; Fukushima, 1998; Fukushima, 1999). But it would be not easy nor straightforward to understand why these spike-like features occur only in  $e_0 = 0.4$  systems, and why the spikes can work as not only to decrease the errors but also to increase



**Figure 12.** An example of the numerical error in the mean anomaly of the middle sized planet when  $e_0 = 0.1$ .  $l_0$  denotes the initial mean longitude of Jupiter. The unit of the vertical axis is deg/year, and the unit of the horizontal axis is year.

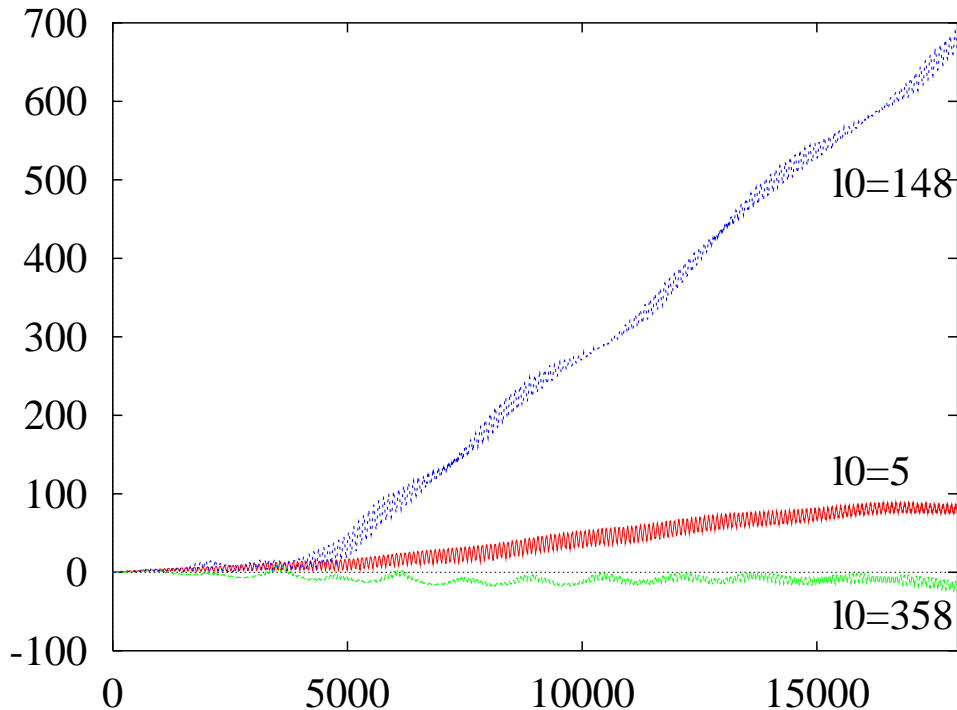


**Figure 13.** An example of the numerical error in the mean anomaly of the middle sized planet when  $e_0 = 0.4$ .  $l_0$  denotes the initial mean longitude of Jupiter. The units of axes are the same with those of Figure 12.



**Figure 14.** An example of the numerical error in the mean anomaly of the middle sized planet when  $e_0 = 0.6$ . The lower panel is a logarithmic version of the upper one. The units of axes are the same with those of Figure 12.

them (cf. Figure 10). Detailed inspection of what is going on in these spike-like regions and of its dependence on various orbital parameters are necessary to definitely answer our question.



**Figure 15.** Another example of the numerical error in the mean anomaly of the middle sized planet when  $e_0 = 0.4$ , near the spike-like area in Figure 10. The units of axes are the same with those of Figure 12.

## 5.2 A planet around a binary star

When we execute numerical integrations in a dynamical system with a small deviation from a certain integrable system (such as Kepler motion or free rotation of rigid bodies), it is not so efficient and operative to resort to the iterative start in order to reduce the numerical errors in symplectic integrators. When the motion of planet deviates little from Keplerian, we should utilize the standard WH map or its variants and extensions, in which we can use many sophisticated techniques which are easy to implement such as the warm start or the symplectic corrector (Wisdom *et al.*, 1996). But when we take care of a system which is not so close to be integrable, we cannot use the method which supposes near-integrability of the system. We anticipate that the iterative start would have its largest effect in such a far-integrable dynamical system.

From this viewpoint, we already have a good example of such non-integrable dynamical systems: An extrasolar planet orbiting around a binary star system, MACHO-97-BLG-41 (Bennett *et al.*, 1999; Albrow *et al.*, 2000). The planetary system around MACHO-97-BLG-41 was discovered by a gravitational microlensing event. Another planetary system (single planet + single star) was also found around MACHO-96-BLG-35 (Rhie *et al.*, 2000), which is expected



to be a kind of solar system kin comprising a low-mass terrestrial planet and a solar-type star.

As for the planetary system around MACHO-97-BLG-41, the lens system is expected to consist of a planet of about three Jupiter masses orbiting a binary stellar system comprising a late-K dwarf star and an M dwarf star. The stars are separated by  $1 \sim 2$  AU (nominally  $\sim 1.6$  AU in Bennett et al. paper), and the planet is orbiting around them at a distance of about several astronomical unit (nominally 7 AU in Bennett et al. paper). Since binary stars are expected to be much more common in the universe than single stars, it is likely that we find many more of this type of extrasolar planetary systems in the future.

One of the demerits of the extrasolar planet detection by microlensing events is that the accuracy of orbital determination is not so high. This is because it is quite hard and generally impossible for us to re-observe a planetary system which has been found by a microlensing event. We have to determine the orbital elements of planets through a set of observational data covering a very short range. Thus orbital elements of extrasolar planets found by microlensing events should contain large errors. We list the possible range of dynamical parameters of MACHO-97-BLG-41 planetary system which are taken from Bennett et al. (1999) in Table 2.

Distance to the lens	$6.3^{+0.6}_{-1.3}$ kpc
Total mass of the lens	$0.8 \pm 0.4 M_{\odot}$
Mass of the primary star	$M_1 = 0.6 \pm 0.3 M_{\odot}$
Mass of the secondary star	$M_2 = 0.16 \pm 0.08 M_{\odot}$
Mass of the possible planet	$M_3 = 0.033 \pm 0.017 M_{\odot}$ ( $= 3.5 \pm 1.8 M_J$ )
Separation between two stars	$1.5^{+0.1}_{-0.3}$ AU
Distance between planet and the center of mass of the lens	$5.7^{+0.6}_{-1.1}$ AU

**Table 2.** Masses and orbital parameters of MACHO-97-BLG-41 planetary system taken from Bennett et al. (1999).  $M_{\odot}$  is the Sun’s mass, and  $M_J$  is the Jupiter’s mass.

Among the rather uncertain orbital elements of the planetary system, we have chosen a set which is shown in Figure 16: the mass of the primary star  $M_1 = 0.6 M_{\odot}$ , the mass of the secondary star  $M_2 = 0.16 M_{\odot}$ , the mass of the planet  $M_3 = 0.028 M_{\odot} = 3 M_J$ , the separation between two stars is 1.6 AU, and the semimajor axis of the planet in terms of the barycentric frame of the lens system is 6 AU. Since our present integrations for this system are still preliminary, we have fixed the initial eccentricities  $e$ , longitudes of ascending nodes  $\Omega$ , inclinations  $I$ , arguments of perihelion  $\varpi$ , and mean anomalies  $l$  of the secondary star and of the planet as

$$\begin{aligned}
 e_{\text{planet},0} &= 0, & e_{\text{secondary},0} &= 0.1, \\
 I_{\text{planet},0} &= I_{\text{secondary},0} = 0.1 \text{ degrees}, \\
 \varpi_{\text{planet},0} &= \varpi_{\text{secondary},0} = 0, \\
 \Omega_{\text{planet},0} &= \Omega_{\text{secondary},0} = 0, \\
 l_{\text{planet},0} &= 0, & l_{\text{secondary},0} &= 180 \text{ degrees}.
 \end{aligned}$$

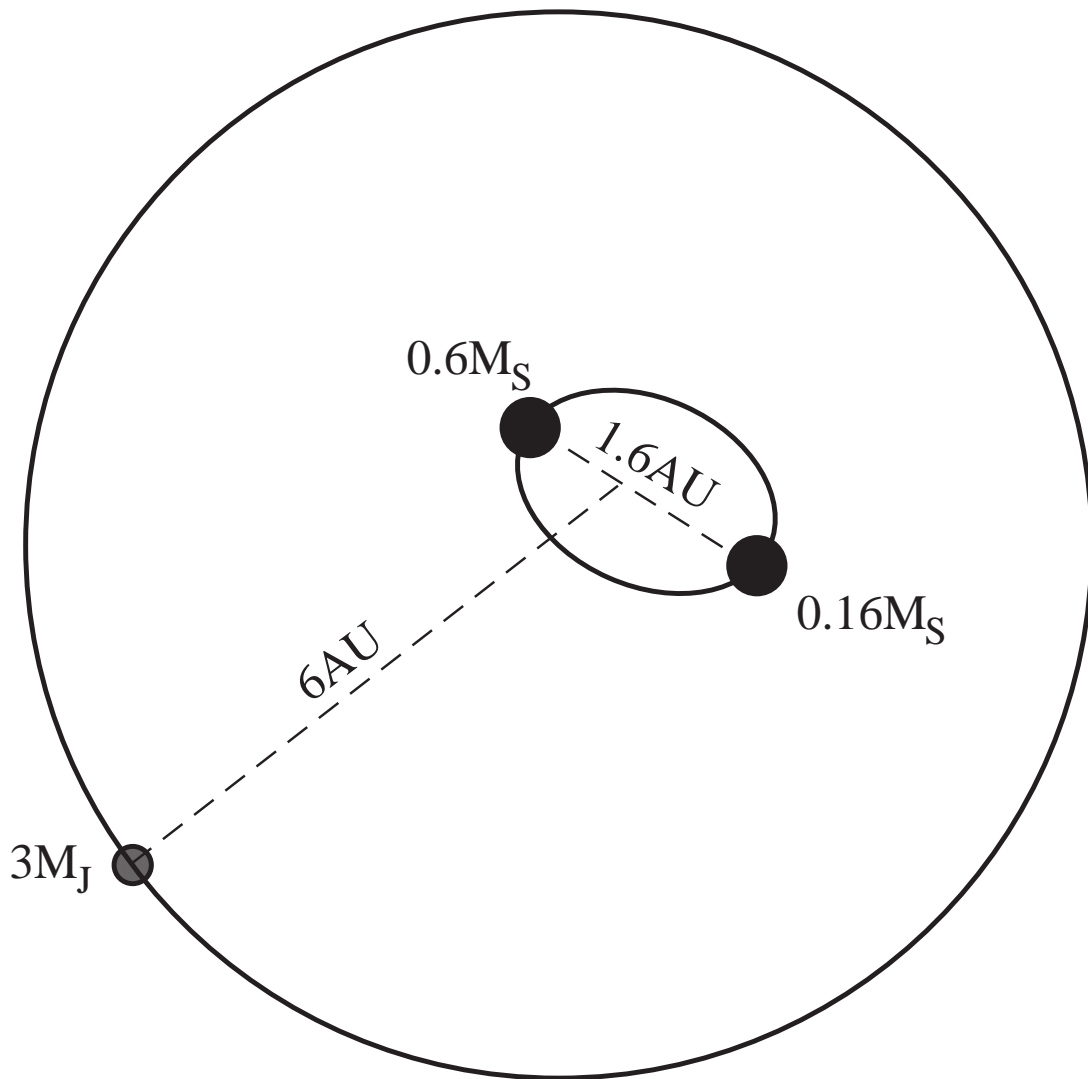
We have selected the non-zero values for inclinations  $I$  so that the system composes a three-dimensional point mass system. By choosing these orbital elements, the ratio of  $\epsilon H_{\text{int}}$  and  $H_{\text{kep}}$  in (141) becomes  $\sim 0.3$ , which is much larger than the perturbed Keplerian motions as described in the previous sections. Thus we think it is worth applying the iterative start when numerically integrating this system.

Several researches have been already done on the dynamical stability of planetary motion in or around binary stars (Wiegert and Holman, 1997; Holman *et al.*, 1997; Mazeh *et al.*, 1997; Holman and Wiegert, 1999). Based on these previous researches, Moriwaki (2001) has investigated on the stability and instability of the MACHO-97-BLG-41 planetary system using a high-order symplectic integrator. Also, Moriwaki and Nakagawa (2002) have performed long-term numerical integrations of the planetary motion with various initial conditions of binary eccentricities, planetary semimajor axis, planetary eccentricity, and longitude of planetary perihelion. The aim of their research was to see which kind of initial configuration produces stable orbits over the whole timespan of their integrations ( $10^6$  binary periods). Their numerical results show that the upper limit of the binary eccentricity in this system is 0.4 when the planet starts from a circular orbit. When the initial eccentricity of the planet becomes large, the stability of the planetary motion is deteriorated. Hence their numerical integration gives us a hint to deduce the upper limit of the initial planetary eccentricity ( $\sim 0.3$  in Moriwaki and Nakagawa’s estimate).

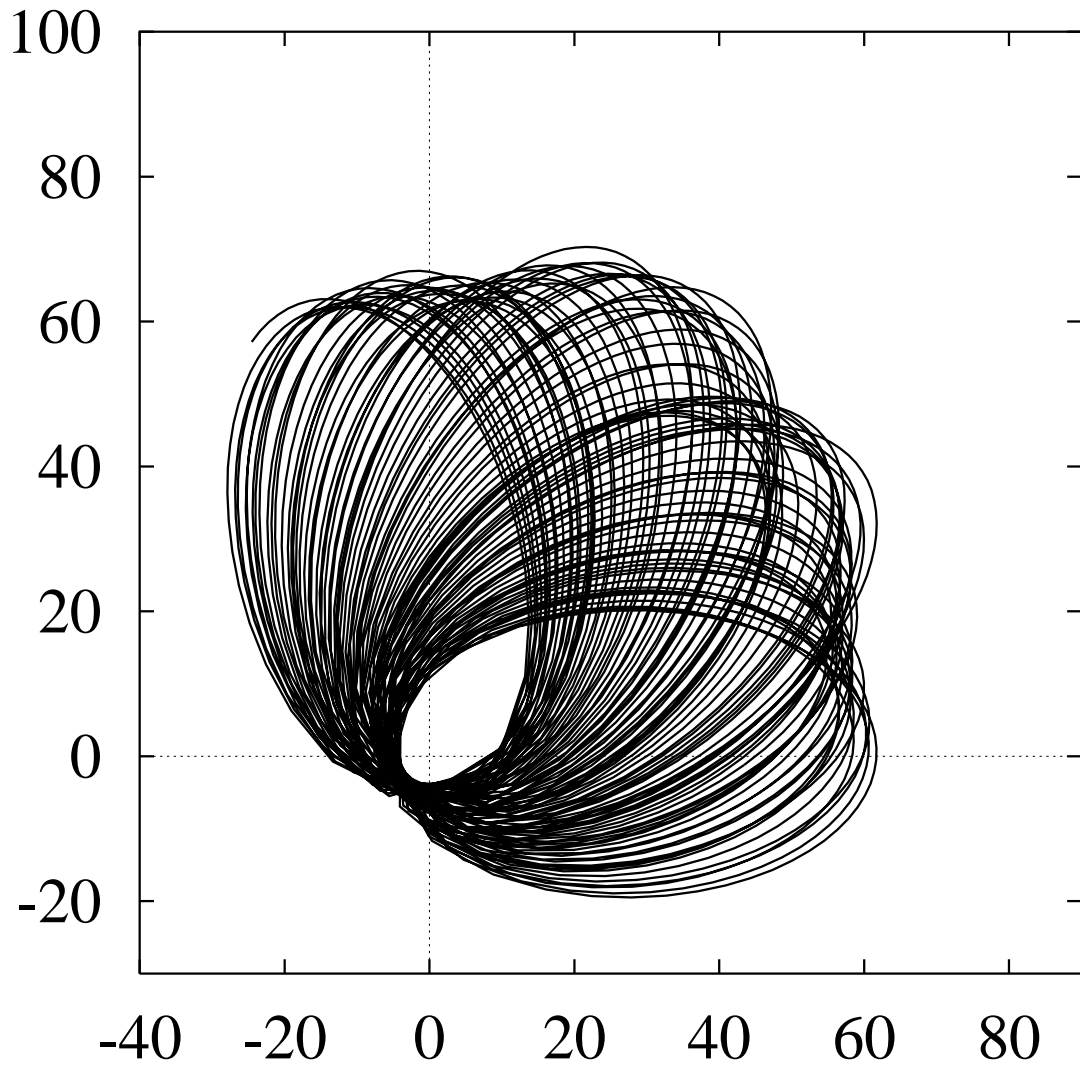
The specific way to implement the iterative start on the planetary system around MACHO-97-BLG-41 is just the same as before:

1. Given a nominal set of initial orbital elements of the planet and the binary stars, we perform an integration with a very high accuracy covering a shorter span than main integrations. We fix the period of this accurate integration as  $2 \times 10^4$  years, similar to the integrations described in the previous section.
2. Choose several initial conditions among the results of the accurate integration for all relevant bodies. We determine the interval of initial conditions for each shorter-term integration as  $P_{\text{planet}}/360$  where  $P_{\text{planet}}$  is the orbital period of the planet around the center of mass of the system. Until the planet gets back to its original longitude, the secondary star rotates around the primary several times.
3. Perform short-term integrations with a normal accuracy using the initial conditions obtained above. We fix the period of this short-term integrations as  $2 \times 10^4$  years. This period should be nearly equal to that of the accurate integration so that we can compare them afterwards.
4. Calculate numerical difference between the accurate and each of the short-term integrations.

In Figure 17 we show the result of the accurate numerical integration of the planetary system around MACHO-97-BLG-41. More specifically speaking, the “accurate” calculation means a numerical integration using a fourth-order generic (TV type) symplectic integrator with a stepsize of 0.0625 days. The planetary orbit rapidly precesses due to the strong perturbation from the binary stars inside. In contrast, we show several examples of the short-term numerical



**Figure 16.** A schematic illustration of the planetary system around MACHO-97-BLG-41 binary. The orbital elements are taken from Table 2.  $M_S$  denotes the Sun's mass ( $= M_\odot$ ).



**Figure 17.** The result of our accurate numerical integration of the planetary system around MACHO-97-BLG-41 binary stars. Eccentricity of the binary stars is 0.1. Only the planetary orbit is drawn here, omitting orbit of the binary stars. The origin of the coordinate is fixed on the center of the mass of the system. The unit of axes is AU.

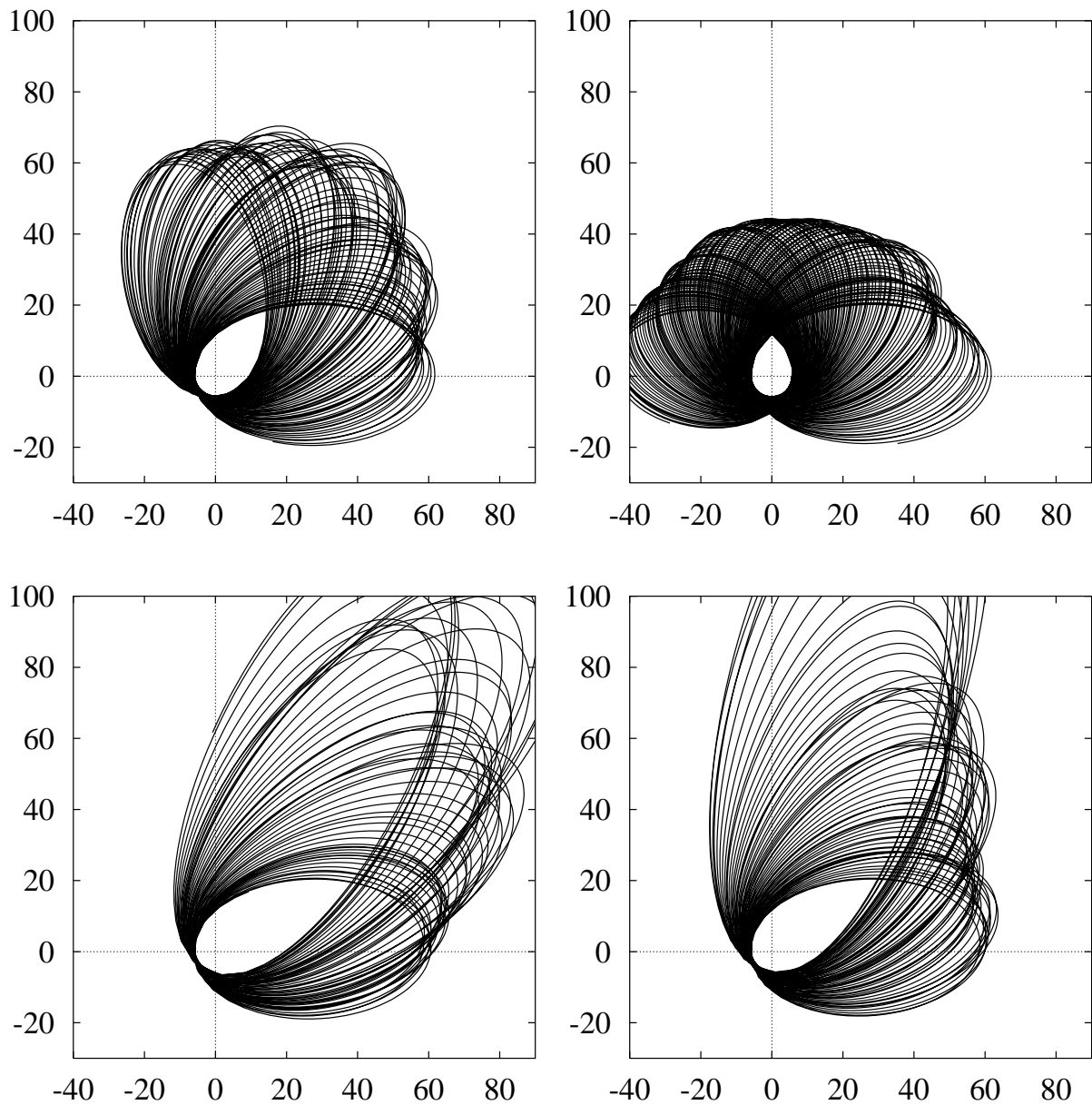
integrations with a moderate accuracy (using the second-order symplectic integrator with a stepsize of 1.0 days) in Figure 18. Although our numerical integrations are still preliminary, we can easily find some very interesting results. Among the short-term numerical integrations, the planetary orbital trajectory is very similar to that of the accurate integration only when  $l_{\text{planet},0} = 16^\circ$ . Other trajectories are quite different, as if each of them shows the orbit in totally different dynamical systems.

There are two possible causes for the above phenomenon. One is the strong dependence of the numerical error in symplectic integrator which we have discussed in the previous sections. Since the disturbance to the planetary orbital motion by the inner binary stars is very large, the “distortion” of the trajectory in phase-space may be remarkable, which leads to the extreme difference in enhancement or reduction of the numerical error shown in Figure 18.

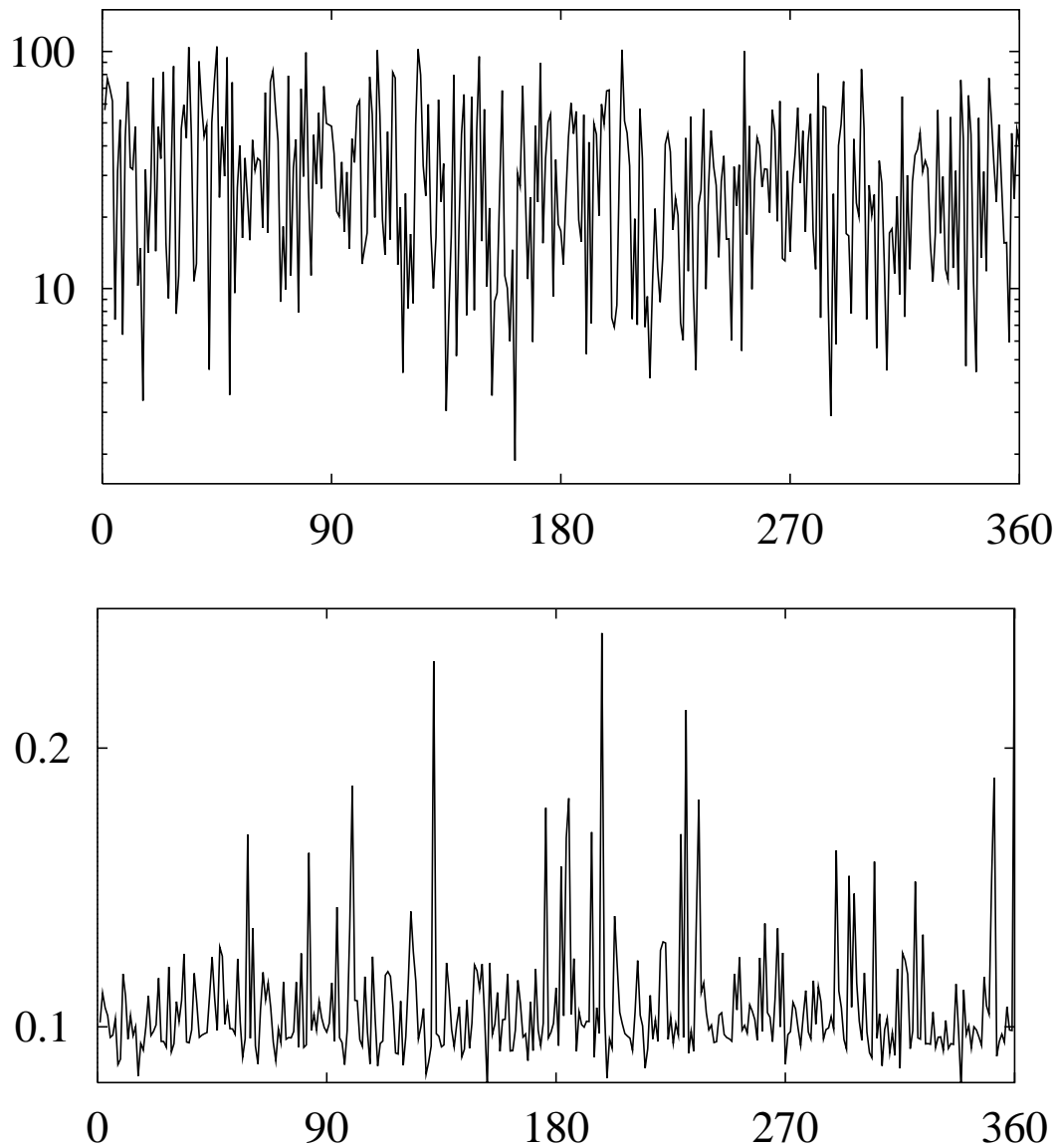
The other reason concerns the reliability of the accurate numerical integration. If the accurate integration is literally “accurate”; that is, exactly expresses the true solution of the differential equation, there is no problem when using the iterative start. The strong dependence of the numerical error such as in Figure 18 can be all ascribed to the difference in the initial orbital positions chosen for the symplectic integration. However, if the accurate integration is not that “accurate”: i.e. if the solution by the accurate integration contains somewhat “inaccurate” compositions compared with the true solution, it is not easy for us to distinguish whether the strong dependence of the numerical error such as in Figure 18 is all due to the difference of chosen initial orbital positions, or due to the chaotic dynamical character which the system involves. In other words, when the accurate integration is not sufficiently accurate, we may be comparing the integration results of many different (and mutually less relevant) dynamical systems, which is not what we meant. Although we have employed a fourth-order symplectic integrator with a relatively smaller stepsize in our accurate integration in Figure 17, the accuracy may not be sufficient. We are now going to confirm the accuracy of our “accurate” integration using ever higher and more precise integration method, such as a sixth- or an eighth-order symplectic integrator with some appropriate start-up procedures.

In Figure 19, we show the relationship between the initial mean longitude of the planet ( $l_{\text{planet},0}$ ) and the RMS numerical errors of the mean longitude and the semimajor axis of the planet using the same procedures as described in the previous sections. We have extracted three examples from the results in Figure 19 and drawn the time evolution of the numerical errors in mean anomalies and semimajor axes in Figures 20 and 21. What we notice first when viewing these figures is the irregularities of lines; we can hardly see any systematic trend in the graphs, unlike when we have taken care of a slightly perturbed three-body system in the previous section. This is we think probably due to the larger perturbation to the planetary orbit by the inner binary stars. We have to check whether this irregular trend is real or not using more accurate numerical integrations.

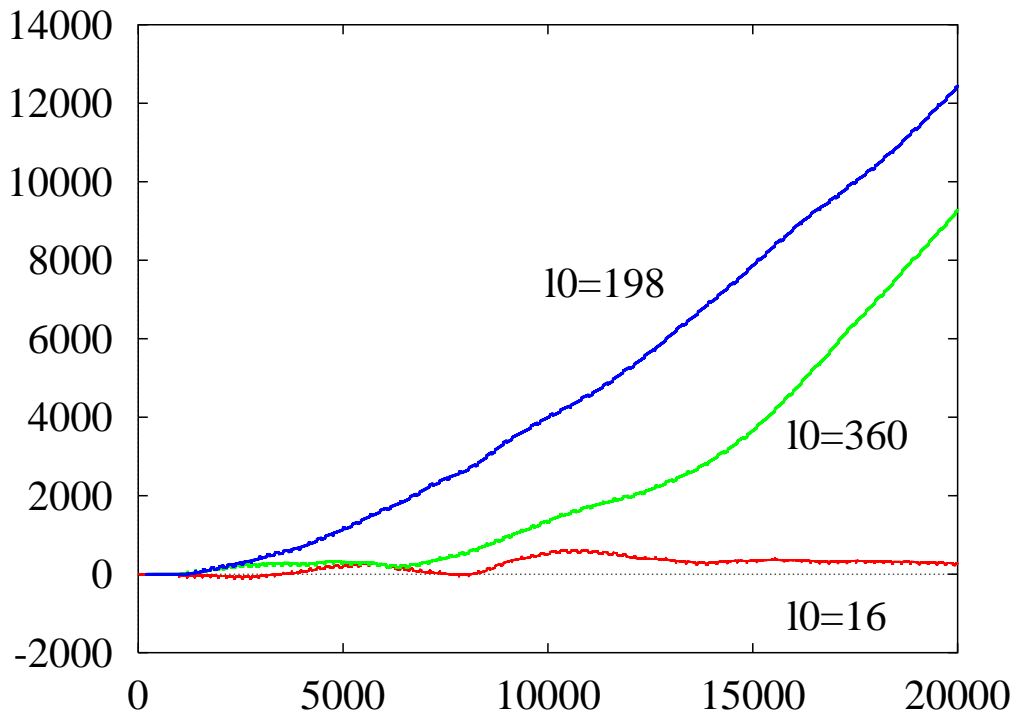
Another difficulty when we adopt the iterative start on a strongly perturbed dynamical system such as the planetary system around MACHO-97-BLG-41 binary stars is related to its non-integrability. A weakly perturbed system such as what we have described in the previous sections is also a non-integrable system, but we call it “nearly integrable.” In nearly-integrable systems, especially those which are close to the superposition of the two-body system, we know that many of angle variables degenerate. Hence there is a considerable difference in the timescale of



**Figure 18.** Some example results of the short-term numerical integrations ( $2 \times 10^4$  years) of the planetary motion around MACHO-97-BLG-41 binary stars when the eccentricity of the binary stars is 0.1. Upper left:  $l_{\text{planet},0} = 16^\circ$ , upper right:  $l_{\text{planet},0} = 34^\circ$ , lower left:  $l_{\text{planet},0} = 198^\circ$ , and lower right:  $l_{\text{planet},0} = 360^\circ$ . Only the planetary orbit is drawn here, omitting the orbit of the binary stars. The origin of the coordinate is fixed on the center of mass of the system. The unit of axes is AU.

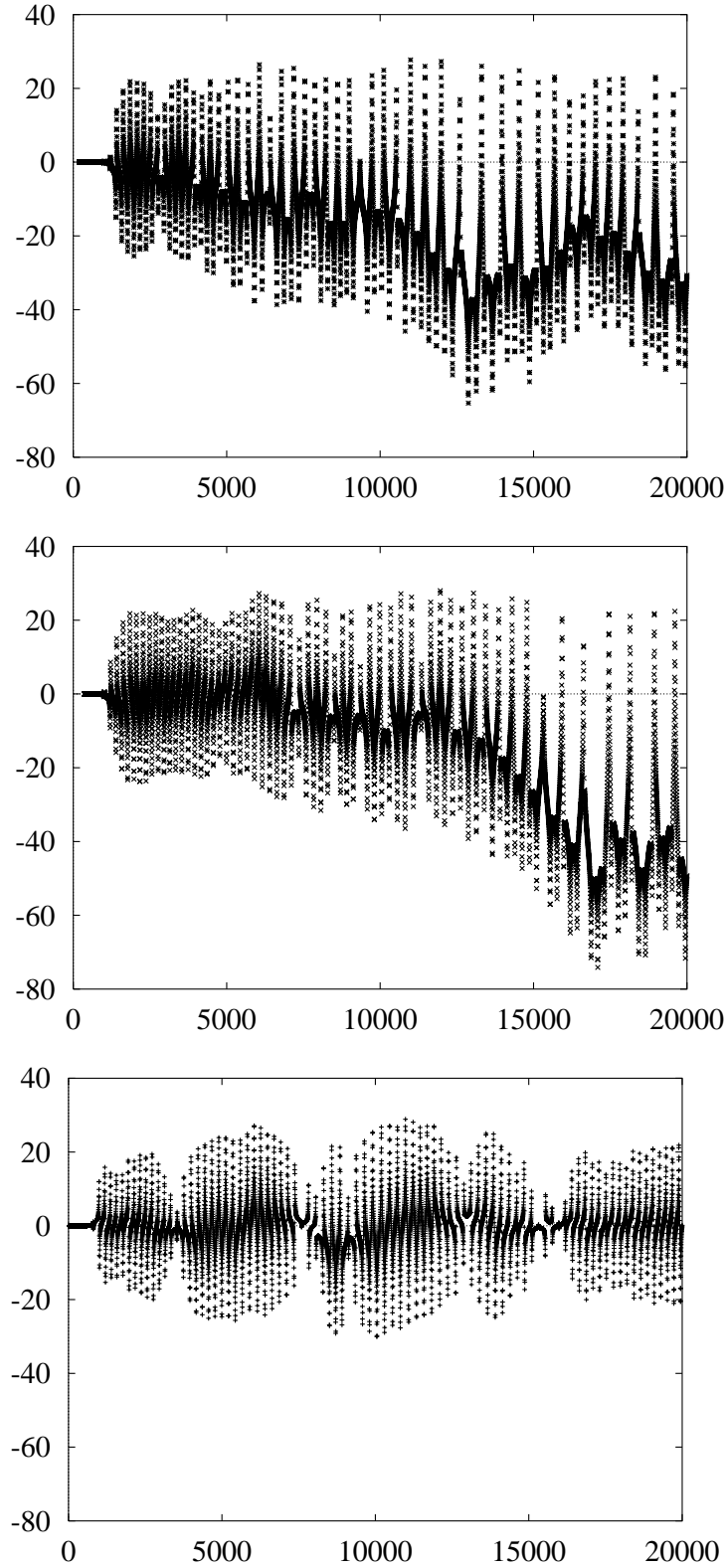


**Figure 19.** The relationship between the initial mean longitude of the planet ( $l_{\text{planet},0}$ ; degree) and the RMS numerical errors of the mean longitude (upper; degree) and semimajor axis (lower; AU) of the planetary orbit in the MACHO-97-BLG-41 system. Each length of numerical data used for the comparison between the accurate and the short-term integrations is  $2 \times 10^4$  years. The origin of the orbital elements is the center of mass of the system.



**Figure 20.** The numerical difference of the planetary mean anomaly in the MACHO-97-BLG-41 system when  $l_{\text{planet},0} = 198^\circ$ ,  $l_{\text{planet},0} = 360^\circ$ , and  $l_{\text{planet},0} = 16^\circ$ . The unit of the vertical axis is degree, and the unit of the horizontal axis is year. The origin of the orbital elements is the center of mass of the system.

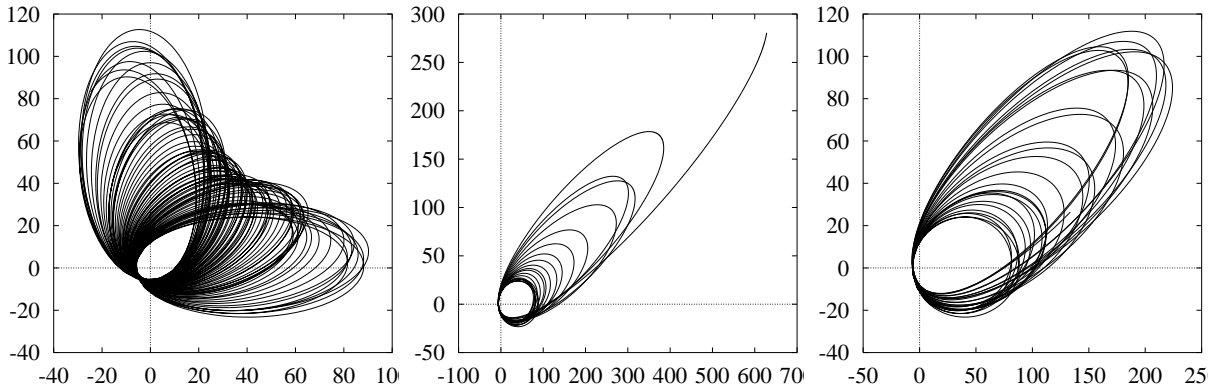




**Figure 21.** The numerical difference of the planetary semimajor axis in the MACHO-97-BLG-41 system: (upper) when  $l_{\text{planet},0} = 198^\circ$ , (middle) when  $l_{\text{planet},0} = 360^\circ$ , (lower) when  $l_{\text{planet},0} = 16^\circ$ . The unit of the vertical axis is AU, and the unit of the horizontal axis is year. The origin of the orbital elements is the center of mass of the system.

each variable in the system. Then it is enough for us to focus on a variable having the shortest timescale in error reduction procedures such as the iterative start (for example, mean anomaly in the Kepler motion). In other words, it is easy for us to guess by which variables we should evaluate numerical errors. However, in strongly perturbed systems such as the planetary system around MACHO-97-BLG-41 binary stars, it is not so easy to determine a variable by which we evaluate numerical errors. As we can see in Figure 18, such a system dose not degenerate any longer, with all angle variables changing quickly. Then, it is not clear whether or not an initial orbital position which reduces the numerical error of one variable also produces the minimum of the numerical error of other variables. In addition, orbits may not be bounded in such a strongly perturbed system: For example, in Figure 22 we show three example results of the “accurate” integrations when the eccentricity of the inner binary stars of MACHO-97-BLG-41 increases to 0.15 from 0.10. We see that the semimajor axis of the planet changes rapidly and secularly, which may indicate that the planetary motion is unbounded and unstable. We think it is still an open question what kind of variable should be used in such systems to reduce the numerical error most efficiently.

As for a planetary system around or inside a binary such as MACHO-97-BLG-41, a dedicated symplectic algorithm developed recently is available (Chambers *et al.*, 2002; Quintana *et al.*, 2002). However, Chambers’ algorithm still exploits the fact that the system is nearly integrable and bounded. If planets goes out or into binary stars, or if the actions of planets change secularly, it is not sure that the dedicated algorithm works as well. The iterative start works possibly well even in such a system keeping the symplecticity, since it is derived from the general-purpose symplectic integrator,  $H = T(p) + V(q)$  type.



**Figure 22.** Three example results of the short-term numerical integrations ( $2 \times 10^4$  years) of the planetary motion around MACHO-97-BLG-41 binary stars when the eccentricity of the binary is 0.15. Left:  $l_{\text{planet},0} = 40^\circ$ , middle:  $l_{\text{planet},0} = 96^\circ$ , and right:  $l_{\text{planet},0} = 221^\circ$ . The unit of axes is AU.

### 5.3 Relationship to the “warm start”

It is meaningful to consider whether there is any relationship between the items in this manuscript and a special start-up procedure called “warm start” (Saha and Tremaine, 1992;

Saha and Tremaine, 1994).

The discussion below follows Saha & Tremaine (1992). As we have seen in the previous sections, Hamiltonian  $\tilde{H}$  for a surrogate system dominating the WH-type symplectic map can be written as follows.

$$\tilde{H} = H + H_{\text{err}}, \quad (140)$$

$$H = H_{\text{kep}} + \epsilon H_{\text{int}}, \quad (141)$$

$$H_{\text{err}} = \frac{\epsilon \tau^2}{24} \{ \{ H_{\text{kep}}, H_{\text{int}} \}, H_{\text{kep}} \} + O(\epsilon^2 \tau^2). \quad (142)$$

We define the actions and the angles in a real system as  $\mathbf{J} = (J_1, J_2, J_3)$  and  $\boldsymbol{\theta} = (\theta_1, \theta_2, \theta_3)$ . Also, the Kepler Hamiltonian  $H_{\text{kep}}$  is described by Delaunay variables as usual  $\mathbf{L} = (L, G, H)$  and  $\mathbf{l} = (l, g, h)$ . Although the Delaunay variables are dedicated to the Kepler motion, the discussion here can be extended to any kind of nearly integrable problems.

We know that the difference between  $H$  and  $H_{\text{kep}}$  is only  $O(\epsilon)$  where  $\epsilon$  is the order of magnitude of the perturbation we consider now. Then we can write as

$$\begin{aligned} J_1 &= L + O(\epsilon), & \theta_1 &= l + O(\epsilon), \\ J_2 &= G + O(\epsilon), & \theta_2 &= g + O(\epsilon), \\ J_3 &= H + O(\epsilon), & \theta_3 &= h + O(\epsilon). \end{aligned} \quad (143)$$

Since  $H_{\text{kep}}$  is a function of  $L$  only (i.e.  $H_{\text{kep}} = -\sum_i \frac{\mu_i^2}{2L_i^2}$ ), all the dependencies of  $H_{\text{kep}}$  on  $J_2, J_3, \theta_1, \theta_2, \theta_3$  are restricted to  $O(\epsilon)$ . Then we get

$$\frac{\partial H_{\text{kep}}}{\partial J_2} = O(\epsilon), \quad \frac{\partial H_{\text{kep}}}{\partial J_3} = O(\epsilon), \quad (144)$$

$$\frac{\partial H_{\text{kep}}}{\partial \theta_1} = O(\epsilon), \quad \frac{\partial H_{\text{kep}}}{\partial \theta_2} = O(\epsilon), \quad \frac{\partial H_{\text{kep}}}{\partial \theta_3} = O(\epsilon). \quad (145)$$

Substituting (144) and (145) into (142) and evaluating the Poisson bracket  $\{, \}$  by canonical variables of the real system  $(\mathbf{J}, \boldsymbol{\theta})$ , we can rewrite the error Hamiltonian  $H_{\text{err}}$ . Then we immediately find that only a term including  $\frac{\partial H_{\text{kep}}}{\partial J_1}$  remains up to  $O(\epsilon)$  approximation since the error Hamiltonian  $H_{\text{err}}$  originally has a factor  $\epsilon$  (142).

$$H_{\text{err}} = -\frac{\epsilon \tau^2}{24} \left( \frac{\partial H_{\text{kep}}}{\partial J_1} \right)^2 \left( \frac{\partial^2 H_{\text{int}}}{\partial \theta_1^2} \right) + O(\epsilon^2 \tau^2). \quad (146)$$

Here we are supposed to concern only bounded motions such as a stable planetary dynamics or a rotational motion of planet. Then,  $\frac{\partial^2 H_{\text{int}}}{\partial \theta_1^2}$  in (146) consists of only periodic terms: if there is a constant term in  $\frac{\partial^2 H_{\text{int}}}{\partial \theta_1^2}$ , e.g.  $C_1$  as

$$\frac{\partial^2 H_{\text{int}}}{\partial \theta_1^2} = C_1, \quad (147)$$

which leads to

$$\frac{\partial H_{\text{int}}}{\partial \theta_1} = C_1 \theta_1 + C_2, \quad (148)$$

where  $C_2$  is another constant of integration. Let us define  $J_{1,H_{\text{int}}}$  as an action due to  $H_{\text{int}}$ . Then, from (148),

$$\frac{dJ_{1,H_{\text{int}}}}{dt} = -\frac{\partial H_{\text{int}}}{\partial \theta_1} = -C_1\theta_1 - C_2, \quad (149)$$

$$\therefore J_{1,H_{\text{int}}} = -C_2t + f(\theta_1; t), \quad (150)$$

where  $f(\theta_1; t)$  is a function of  $\theta_1$  and  $t$ . Equation (150) means that there appears a secular motion in the action  $J_{1,H_{\text{int}}}$  if there is a constant term in  $\frac{\partial^2 H_{\text{int}}}{\partial \theta_1^2}$  in (146), which leads to a possible secular collapse of the system. Thus  $\frac{\partial^2 H_{\text{int}}}{\partial \theta_1^2}$  in (146) must consist of only periodic terms. The fact that  $\frac{\partial^2 H_{\text{int}}}{\partial \theta_1^2}$  is expressed only by periodic terms indicates that there are no “raw” angles  $\theta$  in the disturbing function which describes planetary perturbation. All of the angles appear as the form of periodic functions such as  $\sin \theta$  or  $\cos \theta$ .

From (146), we can decompose the error Hamiltonian  $H_{\text{err}}$  into the superposition of Fourier components as

$$H_{\text{err}} = \epsilon\tau^2 \sum_{\mathbf{m}} X_{\mathbf{m}}(\mathbf{J}) e^{i\mathbf{m}\cdot\boldsymbol{\theta}} + O(\epsilon^2\tau^2), \quad (151)$$

where  $\mathbf{m} = (m_1, m_2, m_3)$  is a integer vector and each  $m_j$  takes any value from  $-\infty$  to  $+\infty$ , and  $X_{\mathbf{m}}$  is the coefficients of Fourier transformation. Since  $H_{\text{err}}$  has no secular term other than  $O(\epsilon^2\tau^2)$ , and since only  $\theta_1$  is directly related to time,  $X_{\mathbf{m}}$  should be zero when  $m_1 = 0$ . Hence the time-averaged (i.e. secular) value of  $H_{\text{err}}$  should be

$$\langle H_{\text{err}} \rangle = O(\epsilon^2\tau^2). \quad (152)$$

The fact described by (152) plays an essential role in the principle of the warm start.

If we define the canonical frequency of the real system  $H$  as

$$\boldsymbol{\omega} \equiv \frac{\partial H}{\partial \mathbf{J}}, \quad (153)$$

the formal solution for the action would be

$$\tilde{\mathbf{J}} = \mathbf{J} - \epsilon\tau^2 \sum_{\mathbf{m}} \frac{X_{\mathbf{m}}\mathbf{m}}{\boldsymbol{\omega} \cdot \mathbf{m}} e^{i\mathbf{m}\cdot\boldsymbol{\theta}}, \quad (154)$$

and the canonical frequency of the surrogate system  $\tilde{H}$  becomes

$$\begin{aligned} \tilde{\boldsymbol{\omega}}(\tilde{\mathbf{J}}) &\equiv \frac{\partial \tilde{H}(\tilde{\mathbf{J}})}{\partial \tilde{\mathbf{J}}} = \frac{\partial}{\partial \tilde{\mathbf{J}}} \left( H(\tilde{\mathbf{J}}) + \langle H_{\text{err}}(\tilde{\mathbf{J}}) \rangle \right) \\ &= \frac{\partial H(\tilde{\mathbf{J}})}{\partial \tilde{\mathbf{J}}} + O(\epsilon^2\tau^2) \\ &= \boldsymbol{\omega}(\tilde{\mathbf{J}}) + O(\epsilon^2\tau^2). \end{aligned} \quad (155)$$

The fundamental idea of the warm start described in Saha & Tremaine (1992) is to make the difference between  $\tilde{\mathbf{J}}$  and  $\mathbf{J}$  as small as possible at the start of symplectic integration, and keep the difference small all through the integration using the adiabatic invariant character of Hamiltonian systems.

Thus we can understand that the warm start is effective only when the error Hamiltonian consists only of periodic terms as in (151), and when its averaged value becomes far smaller

(as in (152)). In this case, the warm start is more effective and easier to implement than the iterative start. However, when the error Hamiltonian does not consist only of periodic terms such as in (48), the warm start is no longer valid. We have to resort to other general method, such as the iterative start.

## 6. Interpretation and other analytical examples

As discussed above, we can reduce the numerical error of  $H = T(p) + V(q)$  type symplectic integrator by choosing certain starting conditions. But mostly, the numerical error does not decrease significantly (cf. when  $e_0 = 0.1$  in Figure 10). What is the difference between systems where we can and cannot reduce the numerical error of the symplectic integrator?

To answer this question, we have applied a canonical perturbation theory to several simple dynamical problems. We consider a symplectic integrator dominated by a surrogate Hamiltonian  $\tilde{H} = H + H_{\text{err}}$  as a kind of nearly-integrable, disturbed Hamiltonian problem. If the Hamiltonian of the real system  $H$  is integrable (e.g. the Kepler motion or the harmonic oscillator) and  $H_{\text{err}}$  is sufficiently small, we can obtain approximate solution of the system, i.e. numerical solution by symplectic integrator including numerical errors.

Suppose the surrogate Hamiltonian takes the following form:

$$\tilde{H}(\theta, J) = H(J) + H_{\text{err}}(\theta, J), \quad (156)$$

where  $\theta$  and  $J$  are the angle and action variables of the real system,  $H$ .  $J$  is an integral (or constant) in  $H$ , hence  $H$  includes no angle,  $\theta$ .  $J$  would be no longer a constant (nor action) in the surrogate system  $\tilde{H}$ , but  $J$  and  $\theta$  still serve as canonical variables in the surrogate system as  $\tilde{H}(\theta, J)$ .

Here we suppose that the degree of freedom of the system is one for simplicity. Extension to problems with larger degrees of freedom is in principle possible, though it generally requires formidable algebra. Since we focus ourselves on a first-order solution here, using a traditional theory (von Zeipel, 1916) or a standard theory exploiting Lie series (Hori, 1966; Deprit, 1969) makes no difference.

Averaging  $H_{\text{err}}$  by the angle  $\theta$ , we obtain the new Hamiltonian  $\tilde{H}^*$  in general as

$$\tilde{H}^*(J^*) = H^*(J^*) + \langle H_{\text{err}}(\theta^*, J^*) \rangle \quad (157)$$

$$= H^*(J^*) + H_{\text{err}}^*(J^*). \quad (158)$$

Then we get the canonical equations of motion for the new system as

$$\frac{dJ^*}{dt} = -\frac{\partial \tilde{H}^*(J^*)}{\partial \theta^*}, \quad (159)$$

$$\begin{aligned} \frac{d\theta^*}{dt} &= \frac{\partial \tilde{H}^*}{\partial J^*} \\ &= \frac{\partial H^*(J^*)}{\partial J^*} + \frac{\partial H_{\text{err}}^*(J^*)}{\partial J^*}, \end{aligned} \quad (160)$$

but since  $\tilde{H}^*$  includes only  $J^*$  and does not include the angle variable  $\theta^*$ ,  $J^*$  is a constant (or an integral) and  $\theta^*$  exhibits a equi-velocity linear motion in phase-space as

$$J^* = \text{constant}, \quad \theta^* = \omega t + \text{constant}, \quad (161)$$

where  $\omega$  is the canonical frequency of the new system defined as

$$\omega(J^*) \equiv \frac{\partial \tilde{H}^*(J^*)}{\partial J^*}. \quad (162)$$

In the following subsections, we take several simple Hamiltonian systems as examples, and see how the solution (i.e. the numerical solution by the symplectic integrator) would be by the canonical perturbation theory.

## 6.1 Harmonic oscillator

Let us begin with the simplest system, the harmonic oscillator with one degree of freedom. The Hamiltonian of the system is

$$H = T(p) + V(q) = \frac{p^2}{2m} + \frac{m\omega_0^2}{2}q^2, \quad (163)$$

where  $q$  and  $p$  are canonical coordinate and momentum.  $\omega_0$  is a constant which describes the oscillation frequency of the system, and  $m$  corresponds to the mass of the oscillator. The angle/action variables  $(\theta, J)$  of the harmonic oscillator are obtained, for example, through the Poincaré transformation as

$$q = \sqrt{\frac{2J}{m\omega_0}} \sin \theta, \quad p = \sqrt{2m\omega_0 J} \cos \theta. \quad (164)$$

The Hamiltonian (163) becomes now

$$H = \omega_0 J. \quad (165)$$

Thus we found the system integrable.

### 6.1.1 Numerical errors of the first-order formula

According to the BCH formula, the error Hamiltonian of the first-order symplectic integrator becomes as follows:

$$H_{\text{err}} = \frac{\tau}{2} \{V, T\} + \frac{\tau^2}{12} (\{\{T, V\}, V\} + \{\{V, T\}, T\}) + O(\tau^3), \quad (166)$$

where  $\tau$  is the stepsize of integration. Each Poisson bracket becomes

$$\begin{aligned} \{V, T\} &= \frac{\partial T}{\partial q} \frac{\partial V}{\partial p} - \frac{\partial T}{\partial p} \frac{\partial V}{\partial q} \\ &= -\omega_0^2 qp \\ &= -\omega_0^2 J \sin 2\theta, \end{aligned} \quad (167)$$

$$\{T, V\} = \omega_0^2 qp = \omega_0^2 J \sin 2\theta, \quad (168)$$

$$\begin{aligned} \{\{T, V\}, V\} &= \left\{ \omega_0^2 qp, \frac{m\omega_0^2}{2} q^2 \right\} \\ &= -m\omega_0^4 q^2 \\ &= -2\omega_0^3 J \sin^2 \theta, \end{aligned} \quad (169)$$

$$\begin{aligned} \{\{V, T\}, T\} &= \left\{ -\omega_0^2 qp, \frac{p^2}{2m} \right\} \\ &= -\frac{\omega^2 p^2}{m} \\ &= -2\omega_0^3 J \cos^2 \theta. \end{aligned} \quad (170)$$

Hence

$$\begin{aligned} H_{\text{err}} &= \frac{\tau}{2} \{V, T\} + \frac{\tau^2}{12} (\{\{T, V\}, V\} + \{\{V, T\}, T\}) + O(\tau^3) \\ &= -\frac{\tau}{2} \omega_0^2 J \sin 2\theta + \frac{\tau^2}{12} (-2\omega_0^3 J \sin^2 \theta - 2\omega_0^3 J \cos^2 \theta) + O(\tau^3) \\ &= -\frac{\tau}{2} \omega_0^2 J \sin 2\theta - \frac{\tau^2}{12} \omega_0^3 J + O(\tau^3). \end{aligned} \quad (171)$$

Hereafter we write the Hamiltonian  $\tilde{H} = H + H_{\text{err}}$  for simplicity as

$$H(\theta, J) = H_0(\theta, J) + H_1(\theta, J), \quad (172)$$

according to the way in the previous section (see (77)).

Then we get

$$H(\theta, J) = \omega_0 J - \frac{\tau}{2} \omega_0^2 J \sin 2\theta - \frac{\tau^2}{12} \omega_0^3 J + O(\tau^3). \quad (173)$$

We transform the original Hamiltonian  $H(\theta, J)$  into an integrable form  $H^*(J^*)$  through a canonical transformation. If we assume that the new Hamiltonian  $H^*$  would be expanded into the form

$$H^*(J^*) = H_0^*(J^*) + H_1^*(J^*) + H_2^*(J^*) + \dots, \quad (174)$$

and the generating function  $S$  of the transformation could be the form

$$S(\theta^*, J^*) = S_0(\theta^*, J^*) + S_1(\theta^*, J^*) + S_2(\theta^*, J^*) + \dots, \quad (175)$$

where the order of magnitude of  $H_{i+1}/H_i$  and  $S_{i+1}/S_i$  ( $i = 0, 1, \dots$ ) equals to that of the perturbation, i.e.  $O(\tau)$ .

Omitting all the algebra on the way, we would obtain

$$H_0^*(J^*) = H_0(J^*) = \omega_0 J^*, \quad (176)$$

hence the zeroth-order Hamiltonian is uniquely determined. As for the first-order Hamiltonian,

$$H_1^*(J^*) = \{H_0(\theta^*, J^*), S_0(\theta^*, J^*)\} + H_1(\theta^*, J^*). \quad (177)$$

Here we have to determine both  $H_1^*(J^*)$  and  $S_0(\theta^*, J^*)$  simultaneously. Thus we request  $H_1^*(J^*)$  not to contain any angle variables as

$$H_1^*(J^*) = \langle H_1(\theta^*, J^*) \rangle_{\theta^*}, \quad (178)$$

and let  $S_0$  include the rest of periodic terms as

$$\{H_0(\theta^*, J^*), S_1(\theta^*, J^*)\} = \langle H_1(\theta^*, J^*) \rangle_{\theta^*} - H_1(\theta^*, J^*). \quad (179)$$

Now let us remember the canonical equations of motion for unperturbed part of the Hamiltonian in the transformed system

$$\frac{d\theta^*}{dt^*} = \frac{\partial H_0}{\partial J^*}, \quad \frac{dJ^*}{dt^*} = -\frac{\partial H_0}{\partial \theta^*}, \quad (180)$$

where  $t^*$  is the “time” for this system. Using (180), the Poisson bracket in (177) becomes

$$\begin{aligned} \{H_0(\theta^*, J^*), S_0(\theta^*, J^*)\}_{(\theta^*, J^*)} &= \frac{\partial H_0}{\partial \theta^*} \frac{\partial S_0}{\partial J^*} - \frac{\partial H_0}{\partial J^*} \frac{\partial S_0}{\partial \theta^*} \\ &= -\left( \frac{\partial S_0}{\partial J^*} \frac{dJ^*}{dt^*} + \frac{\partial S_0}{\partial \theta^*} \frac{d\theta^*}{dt^*} \right) \\ &= -\frac{dS_0}{dt^*}. \end{aligned} \quad (181)$$

Thus (179) becomes

$$\frac{dS_0}{dt^*} = -\{H_0(\theta^*, J^*), S_0(\theta^*, J^*)\} = H_1(\theta^*, J^*) - \langle H_1(\theta^*, J^*) \rangle_{\theta^*}, \quad (182)$$

$$\therefore S_0 = \int (H_1 - H_1^*). \quad (183)$$

Substituting the specific form of  $H_1$  (173) into (178), we obtain

$$\begin{aligned} H_1^*(J^*) &= \left\langle -\frac{\tau}{2}\omega_0^2 J^* \sin 2\theta^* - \frac{\tau^2}{12}\omega_0^3 J^* \right\rangle_{\theta^*} + O(\tau^3) \\ &= -\frac{\tau^2}{12}\omega_0^3 J^* + O(\tau^3). \end{aligned} \quad (184)$$

The final Hamiltonian up to the first-order approximation is thus

$$H^*(J^*) = H_0^*(J^*) + H_1^*(J^*) = \omega_0 J^* - \frac{\tau^2}{12}\omega_0^3 J^* + O(\tau^3). \quad (185)$$

The canonical equations of motion for  $(\theta^*, J^*)$  system are

$$\frac{d\theta^*}{dt} = \frac{\partial H^*(J^*)}{\partial J^*} = \omega_0 - \frac{\tau^2}{12}\omega_0^3, \quad (186)$$

and

$$\frac{dJ^*}{dt} = -\frac{\partial H^*(J^*)}{\partial \theta^*} = 0. \quad (187)$$

Thus  $J^*$  is a constant, and the canonical frequency of the new system  $\omega(J^*)$  becomes

$$\omega(J^*) \equiv \frac{\partial H^*(J^*)}{\partial J^*} = \dot{\theta}^* = \omega_0 - \frac{\tau^2}{12}\omega_0^3, \quad (188)$$



which is also a constant. Since the relationship between the new and old variable has the form

$$\theta = \theta^* + \text{periodic terms}, \quad J = J^* + \text{periodic terms}, \quad (189)$$

the secular numerical error in the angle  $\theta$  is produced from the second term in the right-hand side of (188),  $-\frac{\tau^2}{12}\omega_0^3$ , which is a constant. In this sense, we cannot manage to reduce the secular numerical error of the angle  $\theta$  when we solve the motion of the harmonic oscillator by the first-order symplectic integrator; the error does not depend on initial starting conditions.

### 6.1.2 Numerical errors of the second-order formula

The error Hamiltonian of the second-order symplectic integrator can be obtained by the BCH formula up to  $O(\tau^2)$  as

$$H_{\text{err}} = \frac{\tau^2}{12} \left( \{\{T, V\}, V\} - \frac{1}{2} \{\{V, T\}, T\} \right). \quad (190)$$

We have already calculated the Poisson brackets  $\{\{T, V\}, V\}$  and  $\{\{V, T\}, T\}$ , so

$$\begin{aligned} \frac{12}{\tau^2} H_{\text{err}} &= \{\{T, V\}, V\} - \frac{1}{2} \{\{V, T\}, T\} \\ &= m\omega_0^4 q^2 - \frac{\omega_0^2 p^2}{m} \\ &= m\omega_0^4 \left( \frac{2J}{m\omega_0} \right) \sin^2 \theta - \frac{\omega_0^2}{2m} (2m\omega_0 J) \cos^2 \theta \\ &= 2\omega_0^3 J \sin^2 \theta - \omega_0^3 J \cos^2 \theta \\ &= \frac{\omega_0^3 J}{2} (1 - 3 \cos 2\theta). \end{aligned} \quad (191)$$

Averaging this error Hamiltonian, we obtain

$$H_1^*(J^*) = \langle H_{\text{err}}(\theta^*, J^*) \rangle = \frac{\tau^2 \omega_0^3 J^*}{24}, \quad (192)$$

which leads us to the final Hamiltonian as

$$H^*(J^*) = H_0^*(J^*) + H_1^*(J^*) = \omega_0 J^* + \frac{\tau^2}{24} \omega_0^3 J^* + O(\tau^4). \quad (193)$$

The canonical equations of motion for  $(\theta^*, J^*)$  system are

$$\frac{d\theta^*}{dt} = \frac{\partial H^*(J^*)}{\partial J^*} = \omega_0 + \frac{\tau^2}{24} \omega_0^3 + O(\tau^4), \quad (194)$$

and

$$\frac{dJ^*}{dt} = -\frac{\partial H^*(J^*)}{\partial \theta^*} = 0. \quad (195)$$

Thus  $J^*$  is again a constant, and the canonical frequency of the new system becomes

$$\omega(J^*) \equiv \frac{\partial H^*(J^*)}{\partial J^*} = \dot{\theta}^* = \omega_0 + \frac{\tau^2}{24} \omega_0^3 \quad (196)$$

which is also a constant. Since the relationship between the new and old variable has the form

$$\theta = \theta^* + \text{periodic terms}, \quad J = J^* + \text{periodic terms}, \quad (197)$$

the secular numerical error in the angle  $\theta$  is produced from the second term in the right-hand side of (196),  $\frac{\tau^2}{24}\omega_0^3$ , which is a constant. Thus we know that we cannot reduce the secular numerical error of the angle  $\theta$  arising from the second-order symplectic integrator.

## 6.2 Nonlinear pendulum

As seen before, the harmonic oscillator produces no secular numerical error in the first- and second-order symplectic integrator. We guess this is ascribed to the isochrone character of the potential of the harmonic oscillator—eigenfrequency of the system does not depend on the initial amplitude of oscillation. The eigenfrequency of the harmonic oscillator does not contain action variables;  $\omega_0$  is a pure constant, not a function of action variable such as  $\omega_0(J)$ . The isochrone characteristic is typical of the harmonic oscillator. In contrast, the Keplerian potential,  $-\mu/r$ , is not isochrone. The eigenfrequency of the Keplerian motion (i.e. mean motion  $n$ ) depends on the initial amplitude of oscillation (i.e. semimajor axis  $a$ ) as  $n = \sqrt{\mu/a^3}$ . We already knew that the Keplerian motion produces the secular numerical error in angle variables when we use a first- and second-order symplectic integrator. In this subsection, we check whether a nonlinear and non-isochrone pendulum causes any secular numerical error in symplectic integrators.

### 6.2.1 Angle and action variables

We begin with the following Hamiltonian

$$H(q, p) = \frac{p^2}{2} + \frac{\omega_0^2 q^2}{2} - \frac{\epsilon q^4}{4!} + \frac{\epsilon^2 q^6}{6!} + \dots \quad (198)$$

which is originally derived from the Hamiltonian of a pendulum having the form of  $H = \frac{p^2}{2} + b \cos q$ , but with a slight modification (Boccaletti and Pucacco, 1998). We recognize  $\epsilon$  as a small and constant parameter. The unperturbed part of the Hamiltonian (198) is

$$H_0(q, p) = \frac{p^2}{2} + \frac{\omega_0^2 q^2}{2}, \quad (199)$$

which is identical to the Hamiltonian of the harmonic oscillator. Since we already knew the relationship between  $(q, p)$  and the action-angle variables  $(\theta, J)$  of the harmonic oscillator as (164), we can rewrite the Hamiltonian (199) as

$$H_0(J) = \omega_0 J, \quad (200)$$

which leads to the new form of the whole Hamiltonian as

$$H(\theta, J) = \omega_0 J - \frac{\epsilon J^2}{16} + \frac{\epsilon^2 J^3}{256\omega_0} + \dots \quad (201)$$

Now we start to obtain the action ( $J^*$ ) for the Hamiltonian system (201) which allows us to write

$$\begin{aligned} H(\theta, J) &= H^*(J^*) \\ &= H_0^*(J^*) + \epsilon H_1^*(J^*) + \epsilon^2 H_2^*(J^*) + \dots, \end{aligned} \quad (202)$$

through the canonical transformation of Hori (1966). Note that we implicitly assume that the Hamiltonian  $H(\theta, J)$  nor  $H^*(J^*)$  does not contain time explicitly,

Let the generating function  $S$  of the transformation  $(\theta, J) \rightarrow (\theta^*, J^*)$  as

$$S(\theta^*, J^*) = S_1(\theta^*, J^*) + \epsilon S_2(\theta^*, J^*) + \epsilon^2 S_3(\theta^*, J^*) + \dots \quad (203)$$

We apply the Lie's expansion theorem to  $H(\theta, J)$ , and get

$$H(\theta, J) = H(\theta^*, J^*) + \epsilon \{H(\theta^*, J^*), S(\theta^*, J^*)\} + \frac{\epsilon^2}{2} \{\{H(\theta^*, J^*), S(\theta^*, J^*)\}, S(\theta^*, J^*)\} + \dots \quad (204)$$

Substituting (201) and (203) into (204), we get

$$\begin{aligned} H(\theta, J) &= H_0(\theta^*, J^*) + \epsilon H_1(\theta^*, J^*) + \epsilon^2 H_2(\theta^*, J^*) + \dots \\ &+ \epsilon \{H_0 + \epsilon H_1 + \epsilon^2 H_2 + \dots, S_1 + \epsilon S_2 + \epsilon^2 S_3 + \dots\} \\ &+ \frac{\epsilon^2}{2} \left\{ \left\{ H_0 + \epsilon H_1 + \epsilon^2 H_2 + \dots, S_1 + \epsilon S_2 + \epsilon^2 S_3 + \dots \right\}, S_1 + \epsilon S_2 + \epsilon^2 S_3 + \dots \right\} + \dots \\ &= H_0(\theta^*, J^*) + \epsilon H_1(\theta^*, J^*) + \epsilon^2 H_2(\theta^*, J^*) + \dots \\ &+ \epsilon \{H_0(\theta^*, J^*), S_1(\theta^*, J^*)\} + \epsilon^2 (\{H_0(\theta^*, J^*), S_2(\theta^*, J^*)\} + \{H_1(\theta^*, J^*), S_1(\theta^*, J^*)\}) \\ &+ \frac{\epsilon^2}{2} \{\{H_0(\theta^*, J^*), S_1(\theta^*, J^*)\}, S_1(\theta^*, J^*)\} + O(\epsilon^3). \end{aligned} \quad (205)$$

Equating the two Hamiltonians  $H(\theta, J)$  and  $H^*(J^*)$ , comparing the terms of each order of  $\epsilon$  in (202) and (205), we obtain the result for  $O(\epsilon^0)$  as

$$H_0^*(J^*) = H_0(J^*) = \omega_0 J^*. \quad (206)$$

For  $O(\epsilon^1)$ , we get

$$H_1^*(J^*) = \{H_0(\theta^*, J^*), H_1(\theta^*, J^*)\} + H_1(\theta^*, J^*). \quad (207)$$

Let us consider the canonical equations of motion of the unperturbed system  $H_0^*(J^*)$ , introducing a time-like variable  $t^*$  as

$$\frac{d\theta^*}{dt^*} = \frac{\partial H_0^*(J^*)}{\partial J^*}, \quad \frac{dJ^*}{dt^*} = -\frac{\partial H_0^*(J^*)}{\partial \theta^*}, \quad (208)$$

$$\therefore J^* = \text{constant}, \quad \theta^* = \omega_0 t^* + \theta_0^*, \quad (209)$$

which leads to

$$\begin{aligned} \{H_0^*(J^*), S_1(\theta^*, J^*)\} &= \frac{\partial H_0^*}{\partial \theta^*} \frac{\partial S_1}{\partial J^*} - \frac{\partial H_0^*}{\partial J^*} \frac{\partial S_1}{\partial \theta^*} \\ &= -\left( \frac{\partial S_1}{\partial J^*} \frac{dJ^*}{dt^*} + \frac{\partial S_1}{\partial \theta^*} \frac{d\theta^*}{dt^*} \right) \\ &= -\frac{dS_1}{dt^*}. \end{aligned} \quad (210)$$

As a rule of usual perturbation theory, we request  $H_1^*(J^*)$  not to contain  $t^*$  as

$$\begin{aligned} H_1^*(J^*) &= \langle H_1(\theta^*, J^*) \rangle_{t^*} \\ &= \frac{1}{T} \int_0^T \left[ -\frac{J^{*2}}{6} \sin^4(\omega_0 t^* + \theta_0^*) \right] dt^* \\ &= \frac{\omega}{2\pi} \int_0^{2\pi} \left[ -\frac{J^{*2}}{6} \sin^4 \theta^* \right] \frac{dt^*}{d\theta^*} d\theta^* \\ &= \frac{\omega_0}{2\pi} \int_0^{2\pi} \left[ -\frac{J^{*2}}{48} \sin^4 \theta^* \right] d\theta^* \\ &= -\frac{J^{*2}}{16}. \end{aligned} \quad (211)$$

The leading term of the generating function  $S_1$  becomes

$$\begin{aligned}
S_1(\theta^*, J^*) &= \int (H_1^* - \langle H_1^* \rangle) dt^* \\
&= \int \frac{dS_1}{dt^*} t^* \\
&= \int \frac{J^{*2}}{12} \left( \cos 2\theta^* - \frac{1}{4} \cos 4\theta^* \right) \frac{d\theta^*}{\omega_0} \\
&= \frac{J^*}{24\omega_0} \left( \sin 2\theta^* - \frac{1}{8} \sin 4\theta^* \right), \tag{212}
\end{aligned}$$

neglecting a constant of integration.

For  $O(\epsilon^2)$  terms, we get

$$\begin{aligned}
H_2^*(J^*) &= \{H_0(\theta^*, J^*), S_2(\theta^*, J^*)\} + \{H_1(\theta^*, J^*), S_1(\theta^*, J^*)\} \\
&+ \frac{1}{2} \{ \{H_0(\theta^*, J^*), S_1(\theta^*, J^*)\}, S_1(\theta^*, J^*) \} + H_2(\theta^*, J^*), \tag{213}
\end{aligned}$$

and we request again

$$H_2^*(J^*) = \langle H_2(\theta^*, J^*) \rangle_{t^*}, \tag{214}$$

and

$$\{H_0^*(J^*), S_2(\theta^*, J^*)\} = -\frac{dS_2}{dt^*}. \tag{215}$$

Thus we can calculate ever higher-order components of  $H_i^*$  and  $S_i$  in similar ways. The new Hamiltonian and canonical frequency of the system up to  $O(\epsilon)$  now become

$$H^*(J^*) = H_0^*(J^*) + \epsilon H_1^*(J^*) = \omega_0 J^* - \epsilon \frac{J^{*2}}{16}. \tag{216}$$

and

$$\omega(J^*) \equiv \frac{\partial H^*(J^*)}{\partial J^*} = \omega_0 - \epsilon \frac{J^*}{8}. \tag{217}$$

The canonical equations of motion written in the new variables are

$$\begin{aligned}
\frac{d\theta^*}{dt} &= \frac{\partial H^*(J^*)}{\partial J^*} \\
&= \omega(J^*) = \text{constant}, \tag{218}
\end{aligned}$$

$$\frac{dJ^*}{dt} = -\frac{\partial H^*(J^*)}{\partial \theta^*} = 0, \tag{219}$$

$$\therefore J^* = \text{constant}. \tag{220}$$

The relationship between old  $(\theta, J)$  and new  $(\theta^*, J^*)$  variables is now explicit using the Poisson bracket operator  $D_S \equiv \{, S\}$  as

$$\begin{aligned}
\theta &= e^{\epsilon D_S} \theta^* \\
&= \theta^* + \epsilon \frac{\partial}{\partial J^*} S(\theta^*, J^*) + \frac{\epsilon^2}{2} \{ \{ \theta^*, S(\theta^*, J^*) \}, S(\theta^*, J^*) \} + \dots, \tag{221}
\end{aligned}$$

$$\begin{aligned}
J &= e^{\epsilon D_S} J^* \\
&= J^* - \epsilon \frac{\partial}{\partial \theta^*} S(\theta^*, J^*) + \frac{\epsilon^2}{2} \{ \{ J^*, S(\theta^*, J^*) \}, S(\theta^*, J^*) \} + \dots. \tag{222}
\end{aligned}$$

Substituting the specific form of  $S_1$  (212) into (221) and (222), we get

$$\theta = \theta^* + \epsilon \frac{J^*}{12\omega_0} \left( \sin 2\theta^* - \frac{1}{8} \sin 4\theta^* \right) + O(\epsilon^2), \quad (223)$$

$$J = J^* - \epsilon \frac{J^*}{24\omega_0} \left( \cos 2\theta^* - \frac{1}{2} \cos 4\theta^* \right) + O(\epsilon^2). \quad (224)$$

Since  $(\theta, J)$  are the angle and action variables in the Hamiltonian system  $H_0$  of the harmonic oscillator, the relationship between  $(q, p)$  and  $(\theta, J)$  has been described in (164). Now in the perturbed system (198),  $(\theta, J)$  are no longer angle/action variables, but are still canonical variables described in (223) and (224). Hence we obtain the final solution  $(q, p)$  for the system (198) by substituting  $\theta$  and  $J$  of (223) and (224) into the  $(q, p)$ - $(\theta, J)$  relationship of the system  $H_0$ , i.e. (164). Thus we get

$$q = \sqrt{\frac{2J^*}{\omega_0} \left[ 1 - \frac{\epsilon J^*}{12\omega_0} \left( \cos 2\theta^* - \frac{1}{4} \cos 4\theta^* \right) \right]} \sin \left[ \theta^* + \frac{\epsilon J^*}{12\omega_0} \left( \sin 2\theta^* - \frac{1}{8} \sin 4\theta^* \right) \right] + O(\epsilon^2), \quad (225)$$

$$p = \sqrt{2J\omega_0 \left[ 1 - \frac{\epsilon J}{12\omega_0} \left( \cos 2\theta - \frac{1}{4} \cos 4\theta \right) \right]} \cos \left[ \theta + \frac{\epsilon J}{12\omega_0} \left( \sin 2\theta - \frac{1}{8} \sin 4\theta \right) \right] + O(\epsilon^2). \quad (226)$$

Hereafter we consider  $(\theta, J)$  as  $(\theta^*, J^*)$ , neglecting the superscript  $*$  attached. Hence we get

$$q = \sqrt{\frac{2J}{\omega_0} \left[ 1 - \frac{\epsilon J}{12\omega_0} \left( \cos 2\theta - \frac{1}{4} \cos 4\theta \right) \right]} \sin \left[ \theta + \frac{\epsilon J}{12\omega_0} \left( \sin 2\theta - \frac{1}{8} \sin 4\theta \right) \right] + O(\epsilon^2), \quad (227)$$

$$p = \sqrt{2J\omega_0 \left[ 1 - \frac{\epsilon J}{12\omega_0} \left( \cos 2\theta - \frac{1}{4} \cos 4\theta \right) \right]} \cos \left[ \theta + \frac{\epsilon J}{12\omega_0} \left( \sin 2\theta - \frac{1}{8} \sin 4\theta \right) \right] + O(\epsilon^2). \quad (228)$$

### 6.2.2 Error Hamiltonian in symplectic integrator

Let us consider a situation where we numerically calculate the solutions of a system dominated by the Hamiltonian (198) up to first-order, namely

$$H(q, p) = \frac{p^2}{2} + \frac{\omega_0^2 q^2}{2} - \frac{\epsilon q^4}{24}. \quad (229)$$

When we write the Hamiltonian as  $H = T(p) + V(q)$ ,

$$T(p) = \frac{p^2}{2}, \quad V(q) = \frac{\omega_0^2 q^2}{2} - \frac{\epsilon q^4}{24}. \quad (230)$$

The error Hamiltonian for the first-order symplectic integrator thus becomes

$$\begin{aligned} H_{\text{err},1\text{st}} &= \frac{\tau}{2} \{V(q), T(p)\} \\ &= \frac{\tau}{2} \frac{\partial V}{\partial q} \frac{\partial T}{\partial p} \\ &= \frac{\tau}{2} \left( \omega_0^2 q - \frac{\epsilon}{6} q^3 \right) p. \end{aligned} \quad (231)$$

By (227),

$$\begin{aligned}
q^3 &= \sqrt{\frac{8J^3}{\omega_0^3}} \sin^3 \theta + O(\epsilon) \\
&= \frac{1}{4} \sqrt{\frac{8J^3}{\omega_0^3}} (3 \sin \theta - \sin 3\theta) + O(\epsilon),
\end{aligned} \tag{232}$$

which leads to

$$\begin{aligned}
\omega_0^2 q - \frac{\epsilon}{6} q^3 &= \sqrt{2J\omega_0^3} \left[ \sin \theta + \frac{\epsilon J}{24\omega_0} \left( \frac{5}{2} \sin \theta + \frac{1}{4} \sin 3\theta \right) \right] - \frac{\epsilon}{6} \frac{1}{4} \sqrt{\frac{8J^3}{\omega_0^3}} (3 \sin \theta - \sin 3\theta) \\
&= \sin \theta \left[ \sqrt{2J\omega_0^2} \left( 1 + \frac{\epsilon J}{24\omega_0} \frac{5}{2} \right) - \frac{\epsilon}{6} \frac{3}{4} \sqrt{\frac{8J^3}{\omega_0^3}} \right] + \sin 3\theta \left[ \sqrt{2J\omega_0^3} \frac{\epsilon J}{24\omega_0} \frac{1}{4} + \frac{\epsilon}{6} \frac{1}{4} \sqrt{\frac{8J^3}{\omega_0^3}} \right] \\
&= \sin \theta \left[ \sqrt{2J\omega_0^3} + \epsilon \left( \frac{5}{48} \sqrt{2J^3\omega_0} - \frac{1}{8} \sqrt{8J^3\omega_0} \right) \right] + \epsilon \sin 3\theta \left( \frac{\sqrt{2J^3\omega_0}}{96} + \frac{1}{24} \sqrt{\frac{8J^3}{\omega_0^2}} \right),
\end{aligned} \tag{233}$$

up to  $O(\epsilon)$ . Thus the error Hamiltonian in (231) becomes

$$\begin{aligned}
\frac{2}{\tau} H_{\text{err,1st}} &= \left( \omega_0^2 q - \frac{\epsilon}{6} q^3 \right) p \\
&= \left[ \sin \theta \left( \sqrt{2J\omega_0^3} + \epsilon \left( \frac{5}{48} \sqrt{2J^3\omega_0} - \frac{1}{8} \sqrt{8J^3\omega_0} \right) \right) + \epsilon \sin 3\theta \left( \frac{\sqrt{2J^3\omega_0}}{96} + \frac{1}{24} \sqrt{\frac{8J^3}{\omega_0^2}} \right) \right] \\
&\quad \times \sqrt{2J\omega_0} \left[ \cos \theta + \frac{\epsilon J}{24\omega_0} \left( \frac{5}{2} \sin \theta + \frac{1}{4} \sin 3\theta \right) \right] \\
&= \sqrt{2J\omega_0} \left\{ \sin \theta \cos \theta \left[ \sqrt{2J\omega_0^3} + \epsilon \left( \frac{5}{48} \sqrt{2J^3\omega_0} - \frac{1}{8} \sqrt{8J^3\omega_0} \right) \right] \right. \\
&\quad + \left. \epsilon \left[ \left( \frac{\sqrt{2J^3\omega_0}}{96} + \frac{1}{24} \sqrt{\frac{8J^3}{\omega_0^2}} \right) \sin 3\theta \cos \theta \right. \right. \\
&\quad \left. \left. + \frac{J}{24\omega_0} \sqrt{2J\omega_0^3} \sin \theta \left( \frac{5}{2} \sin \theta + \frac{1}{4} \sin 3\theta \right) \right] \right\} \\
&= \sqrt{2J\omega_0} \left\{ \frac{1}{2} \sin 2\theta \left[ \sqrt{2J\omega_0^3} + \epsilon \left( \frac{5}{48} \sqrt{2J^3\omega_0} - \frac{1}{8} \sqrt{8J^3\omega_0} \right) \right] \right. \\
&\quad + \left. \epsilon \left[ \left( \frac{\sqrt{2J^3\omega_0}}{96} + \frac{1}{24} \sqrt{\frac{8J^3}{\omega_0^2}} \right) \frac{1}{2} (\sin 4\theta + \sin 2\theta) \right. \right. \\
&\quad \left. \left. + \frac{J}{24\omega_0} \sqrt{2J\omega_0^3} \left( \frac{5}{4} - \frac{5}{4} \cos 2\theta - \frac{1}{8} \cos 4\theta + \frac{1}{8} \cos 2\theta \right) \right] \right\},
\end{aligned} \tag{234}$$

up to  $O(\epsilon)$ . Hence if we average  $H_{\text{err,1st}}$  over  $\theta$ , then we get

$$\begin{aligned}
\langle H_{\text{err,1st}} \rangle &= \epsilon \frac{5}{4} \frac{\tau}{2} \sqrt{2J\omega_0} \frac{J}{24\omega_0} \sqrt{2J\omega_0^3} \\
&= \epsilon \tau \frac{5}{96} \omega_0 J^2.
\end{aligned} \tag{235}$$

In order to estimate the numerical error of the first-order symplectic integrator when adopting to the nonlinear pendulum system, we now apply the Hori's perturbation theory to a Hamiltonian

$$H = \frac{p^2}{2} + \frac{\omega_0^2 q^2}{2} - \frac{\epsilon q^4}{24} + H_{\text{err},1\text{st}}. \quad (236)$$

We rewrite the above Hamiltonian as

$$H = H_0(J) + H_1(\theta, J), \quad (237)$$

where

$$H_0 = \frac{p^2}{2} + \frac{\omega_0^2 q^2}{2} - \frac{\epsilon q^4}{24} = \omega_0 J - \epsilon \frac{J^2}{16}, \quad (238)$$

from (216), and

$$H_1(\theta, J) = H_{\text{err},1\text{st}}(\theta, J), \quad (239)$$

from (234). Since we already knew the averaged perturbation Hamiltonian as (235), applying the perturbation theory gives us a new transformed Hamiltonian as

$$H^*(J^*) = \omega_0 J^* - \epsilon \frac{J^{*2}}{16} + \epsilon \tau \frac{5}{96} \omega_0 J^{*2}, \quad (240)$$

and a new canonical frequency as

$$\omega(J^*) \equiv \frac{\partial H^*(J^*)}{\partial J^*} = \omega_0 - \frac{\epsilon}{8} J^* - \epsilon \tau \frac{5}{192} \omega_0 J^*. \quad (241)$$

Now that the canonical frequency  $\omega$  includes the action  $J^*$  as  $\omega(J^*)$ , we may be able to make it approach the real value,  $\omega_0 - \frac{\epsilon}{8} J_0$  where  $J_0$  is the initial (or ‘‘observed’’) value of the action in real system.

The canonical equation of motion for  $J^*$  becomes as

$$\frac{dJ^*}{dt} = -\frac{\partial H^*(J^*)}{\partial \theta^*}, \quad (242)$$

from which we know that  $J^*$  is a constant. According to the relationship between old and new variables of (222), we get

$$\begin{aligned} J &= e^{\epsilon D_S} J^* \\ &= J^* - \epsilon \frac{\partial}{\partial \theta^*} S(\theta^*, J^*) + \frac{\epsilon^2}{2} \{ \{ J^*, S(\theta^*, J^*) \}, S(\theta^*, J^*) \} \\ &= J^* - \frac{\partial}{\partial \theta^*} \int (H_1 - H_1^*) dt^* \\ &= J^* - \frac{1}{\omega_0} (H_1 - H_1^*). \end{aligned} \quad (243)$$

Suppose  $J = J_0$  when  $t = 0$ , then

$$J_0 = J^* - \frac{1}{\omega_0} (H_{1,t=0} - H_1^*), \quad (244)$$

since  $J^*$  and  $H_1^*$  are constants, so

$$\therefore J^* = J_0 + \frac{1}{\omega_0} (H_{1,t=0} - H_1^*). \quad (245)$$

As for  $\theta^*$ , the canonical equation of motion becomes

$$\begin{aligned}
\frac{d\theta^*}{dt} &= \frac{\partial H^*(J^*)}{\partial J^*} \\
&= \omega_0 - \frac{\epsilon}{8} J^* + \epsilon\tau \frac{5\omega_0}{96} J^* \\
&= \omega_0 - \frac{\epsilon}{8} \left( J_0 + \frac{1}{\omega_0} (H_{1,t=0} - H_1^*) \right) + \epsilon\tau \frac{5\omega_0}{96} \left( J_0 + \frac{1}{\omega_0} (H_{1,t=0} - H_1^*) \right) \\
&= \omega_0 - \frac{\epsilon}{8} J_0 + \left( \epsilon\tau \frac{5\omega_0}{96} - \frac{\epsilon}{8} \right) \frac{H_{1,t=0} - H_1^*}{\omega_0} + \epsilon\tau \frac{5\omega_0}{96} J_0.
\end{aligned} \tag{246}$$

In (246), the first two terms in the right-hand side ( $\omega_0 - \frac{\epsilon}{8} J_0$ ) denote the canonical frequency of the unperturbed Hamiltonian system, (238). Other terms denote numerical secular error of the angle variable,  $\theta$ . What is most important here is that the secular (or constant) numerical error

$$\left( \epsilon\tau \frac{5\omega_0}{96} - \frac{\epsilon}{8} \right) \frac{H_{1,t=0} - H_1^*}{\omega_0} + \epsilon\tau \frac{5\omega_0}{96} J_0, \tag{247}$$

may depend strongly on initial values of  $J$ ,  $\theta$ , and parameters  $\epsilon$ ,  $\tau$ , and  $\omega_0$ . Although we do not demonstrate here, certain combinations of these parameters may reduce the secular error of (247) nearly equal to zero. Other combinations may terribly increase the secular numerical error. This kind of error reduction happens only when the canonical frequency of a Hamiltonian system depends on its initial oscillation amplitude; in other words, when the potential of the Hamiltonian is not isochrone, and dependent on  $J$ . The reduction or non-reduction of the secular numerical error in planetary longitudes seen in the previous sections is thus qualitatively understood to some extent.



## Appendix A. Jacobi coordinate

We request a Hamiltonian used in the WH map to have the following properties:

1. As for the Keplerian part, it should have the same form as the Hamiltonian of the two-body problem,  $\frac{p^2}{2m} - \frac{\mu}{r}$ , or the sum of this form.
2. As for the interaction part, it should be described only by the relative distance, such as  $V(\mathbf{r})$ .
3. The magnitude of the interaction part should be much less than that of the Keplerian part ( $H_{\text{kep}} \gg H_{\text{int}}$ ).

However, simple heliocentric or barycentric coordinate does not satisfy the above requests. For example, writing the Hamiltonian using the barycentric coordinate ends up with

$$\begin{aligned}
H &= \sum_{i=0}^N \frac{\mathbf{p}_i^2}{2m_i} + \left( - \sum_{i=1}^N \frac{Gm_0m_i}{|\mathbf{r}_i - \mathbf{r}_0|} + \sum_{i=1}^N \frac{Gm_0m_i}{|\mathbf{r}_i - \mathbf{r}_0|} \right) - \sum_{i=0}^N \sum_{j=i+1}^N \frac{Gm_im_j}{|\mathbf{r}_i - \mathbf{r}_j|} \\
&= \frac{\mathbf{p}_0^2}{2m_0} + \sum_{i=1}^N \left( \frac{\mathbf{p}_i^2}{2m_i} - \frac{Gm_0m_i}{|\mathbf{r}_i - \mathbf{r}_0|} \right) + \sum_{i=1}^N \frac{Gm_0m_i}{|\mathbf{r}_i - \mathbf{r}_0|} - \left( \sum_{j=1}^N \frac{Gm_0m_j}{|\mathbf{r}_0 - \mathbf{r}_j|} + \sum_{i=1}^N \sum_{j=i+1}^N \frac{Gm_im_j}{|\mathbf{r}_i - \mathbf{r}_j|} \right) \\
&= \frac{\mathbf{p}_0^2}{2m_0} + \sum_{i=1}^N \left( \frac{\mathbf{p}_i^2}{2m_i} - \frac{Gm_0m_i}{|\mathbf{r}_i - \mathbf{r}_0|} \right) - \sum_{i=1}^N \sum_{j=i+1}^N \frac{Gm_im_j}{|\mathbf{r}_i - \mathbf{r}_j|}, \tag{248}
\end{aligned}$$

where we cannot classify the kinetic energy of the Sun ( $\mathbf{p}_0^2/2m_0$ ) into  $H_{\text{kep}}$  nor  $H_{\text{int}}$ . One of the canonical variables which suits our request is the Jacobi coordinates (Plummer, 1960). The Jacobi coordinates  $\tilde{\mathbf{r}}_i$  are defined as

$$\tilde{\mathbf{r}}_i = \mathbf{r}_i - \frac{1}{\sigma_{i-1}} \sum_{j=1}^{i-1} m_j \mathbf{r}_j, \tag{249}$$

where

$$\sigma_i = \sigma_{i-1} + m_i, \quad \sigma_0 = m_0 = M_\odot, \quad \sigma_{-1} \equiv 0, \tag{250}$$

$$\tilde{m}_i = \frac{\sigma_{i-1}}{\sigma_i} m_i, \tag{251}$$

$$\tilde{\mu}_i = \frac{\sigma_i}{\sigma_{i-1}} G, \tag{252}$$

Canonical momenta which are conjugate to  $\tilde{\mathbf{r}}_i$  are

$$\tilde{\mathbf{p}}_i = \tilde{m}_i \tilde{\mathbf{v}}_i, \tag{253}$$

and the velocities are

$$\tilde{\mathbf{v}}_i = \frac{d\tilde{\mathbf{r}}_i}{dt}. \tag{254}$$

In this manuscript, we have utilized the Jacobi coordinate system in our symplectic numerical integration of the  $H = T(p) + V(q)$  type. Thus the discussion below has a certain sense to describe our method of numerical integration in detail.

The advantage of transforming to the Jacobi variables is that in the barycentric frame, the kinetic energy of the  $N + 1$ -body system becomes

$$\sum_{i=1}^N \frac{\tilde{\mathbf{p}}_i^2}{2\tilde{m}_i}, \quad (255)$$

without terms of the central mass as follows (Plummer, 1960).

When we represent the position of the barycenter of the particle of 1 to  $i$  as  $\mathbf{R}_i$ ,

$$\sigma_i \mathbf{R}_i = m_0 \mathbf{r}_0 + m_1 \mathbf{r}_1 + m_2 \mathbf{r}_2 + m_{i-1} \mathbf{r}_{i-1} + m_i \mathbf{r}_i, \quad (256)$$

$$\sigma_{i-1} \mathbf{R}_{i-1} = m_0 \mathbf{r}_0 + m_1 \mathbf{r}_1 + m_2 \mathbf{r}_2 + m_{i-1} \mathbf{r}_{i-1}. \quad (257)$$

Subtracting (257) from (256),

$$\sigma_i \mathbf{X}_i - \sigma_{i-1} \mathbf{X}_{i-1} = m_i \mathbf{r}_i = (\sigma_i - \sigma_{i-1}) \mathbf{r}_i, \quad (258)$$

which is due to the definition of  $\sigma_i$  (250). By the definition of the Jacobi coordinates  $\tilde{\mathbf{r}}_i$ ,

$$\tilde{\mathbf{r}}_i = \mathbf{r}_i - \mathbf{R}_{i-1}, \quad (259)$$

$$\therefore \mathbf{r}_i = \tilde{\mathbf{r}}_i + \mathbf{R}_{i-1}. \quad (260)$$

Substituting (260) into (258),

$$\sigma_i \mathbf{R}_i - \sigma_{i-1} \mathbf{R}_{i-1} = (\sigma_i - \sigma_{i-1})(\tilde{\mathbf{r}}_i + \mathbf{R}_{i-1}), \quad (261)$$

$$\therefore \sigma_i (\mathbf{R}_i - \mathbf{R}_{i-1}) = (\sigma_i - \sigma_{i-1}) \tilde{\mathbf{r}}_i. \quad (262)$$

Hereafter we concentrate on the  $x$ -components of the vectors  $\mathbf{r}_i$ ,  $\tilde{\mathbf{r}}_i$ ,  $\mathbf{R}_i$ :  $x_i$ ,  $\tilde{x}_i$ , and  $X_i$ , respectively. Taking the square of (258) and (262),

$$(\sigma_i - \sigma_{i-1})^2 x_i^2 = (\sigma_i X_i - \sigma_{i-1} X_{i-1})^2, \quad (263)$$

$$(\sigma_i - \sigma_{i-1})^2 \tilde{x}_i^2 = \sigma_i^2 (X_i - X_{i-1})^2. \quad (264)$$

Performing the operation (263) - (264)  $\times \frac{\sigma_{i-1}}{\sigma_i}$ , we get

$$\begin{aligned} & (\sigma_i - \sigma_{i-1})^2 \left( x_i^2 - \frac{\sigma_{i-1}}{\sigma_i} \tilde{x}_i^2 \right) \\ &= (\sigma_i X_i - \sigma_{i-1} X_{i-1})^2 - \frac{\sigma_{i-1}}{\sigma_i} (X_i - X_{i-1})^2 \\ &= \sigma_i^2 X_i^2 - 2\sigma_i \sigma_{i-1} X_i X_{i-1} + \sigma_{i-1}^2 X_{i-1}^2 - \sigma_{i-1} \sigma_i (X_i^2 - 2X_i X_{i-1} + X_{i-1}^2) \\ &= X_i^2 (\sigma_i^2 - \sigma_i \sigma_{i-1}) + X_{i-1}^2 (\sigma_{i-1}^2 - \sigma_i \sigma_{i-1}) \\ &= (\sigma_i - \sigma_{i-1}) (\sigma_i X_i^2 - \sigma_{i-1} X_{i-1}^2). \end{aligned} \quad (265)$$

In the case of finite-mass system,  $\sigma_i \neq \sigma_{i-1}$ , then

$$(\sigma_i - \sigma_{i-1}) \left( x_i^2 - \frac{\sigma_{i-1}}{\sigma_i} \tilde{x}_i^2 \right) = \sigma_i X_i^2 - \sigma_{i-1} X_{i-1}^2. \quad (266)$$

Addition of all the equations of the type (266) from  $i = 0$  to  $i = N$ ,

$$\begin{aligned}
& \sum_{i=0}^N (\sigma_i - \sigma_{i-1}) \left( r_i^2 - \frac{\sigma_{i-1}}{\sigma_i} \tilde{r}_i^2 \right) \\
&= \left( \sigma_0 X_0^2 - \sigma_{-1} X_{-1}^2 \right) + \left( \sigma_1 X_1^2 - \sigma_0 X_0^2 \right) + \left( \sigma_2 X_2^2 - \sigma_1 X_1^2 \right) \\
&\quad + \cdots + \left( \sigma_{N-1} X_{N-1}^2 - \sigma_{N-2} X_{N-2}^2 \right) + \left( \sigma_N X_N^2 - \sigma_{N-1} X_{N-1}^2 \right) \\
&= \sigma_N X_N^2 - \sigma_0 X_0^2 \\
&= \sigma_N X_N^2. \quad (\because \sigma_{-1} = 0)
\end{aligned} \tag{267}$$

Since  $\sigma_i - \sigma_{i-1} = m_i$ ,

$$\begin{aligned}
\sum_{i=0}^N m_i x_i^2 &= \sum_{i=0}^N m_i \frac{\sigma_{i-1}}{\sigma_i} \tilde{x}_i^2 + \sigma_N X_N^2 \\
&= \sum_{i=1}^N m_i \frac{\sigma_{i-1}}{\sigma_i} \tilde{x}_i^2 + \sigma_N X_N^2 \quad (\because \sigma_{-1} = 0) \\
&= \sum_{i=1}^N \tilde{m}_i \tilde{x}_i^2 + \sigma_N X_N^2.
\end{aligned} \tag{268}$$

The relations between the coordinates have been written down for one kind only. But they are linear and the same for all three coordinates  $\mathbf{r}_i = (x_i, y_i, z_i)$ ,  $\tilde{\mathbf{r}}_i = (\tilde{x}_i, \tilde{y}_i, \tilde{z}_i)$ , and  $\mathbf{R}_i = (X_i, Y_i, Z_i)$  separately as

$$\sum_{i=0}^N m_i y_i^2 = \sum_{i=1}^N \tilde{m}_i \tilde{y}_i^2 + \sigma_N Y_N^2, \tag{269}$$

$$\sum_{i=0}^N m_i z_i^2 = \sum_{i=1}^N \tilde{m}_i \tilde{z}_i^2 + \sigma_N Z_N^2. \tag{270}$$

Above derivation can be applied also to the velocity components

$$\mathbf{v}_i = \frac{d\mathbf{r}}{dt} = (\dot{x}_i, \dot{y}_i, \dot{z}_i), \tag{271}$$

$$\tilde{\mathbf{v}}_i = \frac{d\tilde{\mathbf{r}}}{dt} = (\dot{\tilde{x}}_i, \dot{\tilde{y}}_i, \dot{\tilde{z}}_i), \tag{272}$$

$$\mathbf{V}_i = \frac{d\mathbf{R}}{dt} = (\dot{X}_i, \dot{Y}_i, \dot{Z}_i), \tag{273}$$

as

$$\sum_{i=0}^N m_i \dot{x}_i^2 = \sum_{i=1}^N \tilde{m}_i \dot{\tilde{x}}_i^2 + \sigma_N \dot{X}_N^2, \tag{274}$$

$$\sum_{i=0}^N m_i \dot{y}_i^2 = \sum_{i=1}^N \tilde{m}_i \dot{\tilde{y}}_i^2 + \sigma_N \dot{Y}_N^2, \tag{275}$$

$$\sum_{i=0}^N m_i \dot{z}_i^2 = \sum_{i=1}^N \tilde{m}_i \dot{\tilde{z}}_i^2 + \sigma_N \dot{Z}_N^2. \tag{276}$$

Adding (274), (275), (276), we can represent the kinetic energy of the system

$$\sum_{i=0}^N \frac{m_i}{2} (\dot{y}_i^2 + \dot{z}_i^2) = \sum_{i=1}^N \frac{\tilde{m}_i}{2} (\dot{x}_i^2 + \dot{y}_i^2 + \dot{z}_i^2) + \frac{\sigma N}{2} (\dot{X}_N^2 + \dot{Y}_N^2 + \dot{Z}_N^2), \quad (277)$$

or using the momentum  $\mathbf{p}_i$  and  $\tilde{\mathbf{p}}_i$

$$\sum_{i=0}^N \frac{\mathbf{p}_i^2}{2m_i} = \sum_{i=1}^N \frac{\tilde{\mathbf{p}}_i^2}{2\tilde{m}_i} + \frac{\mathbf{p}_R^2}{2M_{\text{tot}}}, \quad (278)$$

where  $\mathbf{p}_R$  is the total momentum of the barycenter (total momentum of the whole system), and  $M_{\text{tot}}$  is the total mass of the system,  $M_{\text{tot}} = \sum_{i=0}^N m_i$ . Then, the general Hamiltonian for the  $N + 1$ -body (one central mass and  $N$  planets) becomes

$$H = \frac{\mathbf{p}_R^2}{2M_{\text{tot}}} + \sum_{i=1}^N \frac{\tilde{\mathbf{p}}_i^2}{2\tilde{m}_i} - \sum_{i=0}^N \sum_{j=i+1}^N \frac{k^2 m_i m_j}{|\mathbf{r}_i - \mathbf{r}_j|}. \quad (279)$$

By construction, the total momentum  $\mathbf{p}_R$  is an integral of the motion, which means that the center of mass moves as a free particle. Hence the center of mass contribution to the Hamiltonian  $\mathbf{p}_R^2/2M_{\text{tot}}$  will be omitted. Thus the problem of  $N + 1$  bodies is reduced to a problem of  $N$  fictitious bodies with mass  $\tilde{m}_i$ , and the total order of the differential equations of motion is reduced by 6. In view of (253) and (254), we can rewrite the full Hamiltonian as

$$\begin{aligned} H &= \sum_{i=1}^N \frac{\tilde{\mathbf{p}}_i^2}{2\tilde{m}_i} - \sum_{i=0}^N \sum_{j=i+1}^N \frac{k^2 m_i m_j}{|\mathbf{r}_i - \mathbf{r}_j|} \\ &= \sum_{i=1}^N \frac{\tilde{\mathbf{p}}_i^2}{2\tilde{m}_i} - \sum_{i=1}^N \frac{k^2 m_i m_0}{r_i} - \sum_{i=1}^N \sum_{j=i+1}^N \frac{k^2 m_i m_j}{|\mathbf{r}_i - \mathbf{r}_j|}. \end{aligned} \quad (280)$$

where  $r_j$  denote the heliocentric distance,  $|\mathbf{r}_i - \mathbf{r}_0|$ . Note that we have changed the index  $j$  to  $i$  for simplicity in the second sum of (280). Adding and subtracting the quantity

$$\sum_{i=1}^N \frac{k^2 m_i m_0}{\tilde{r}_i}, \quad (281)$$

into the righthand-side of (280), the Hamiltonian becomes

$$\begin{aligned} H &= \sum_{i=1}^N \frac{\tilde{\mathbf{p}}_i^2}{2\tilde{m}_i} + \left( - \sum_{i=1}^N \frac{k^2 m_i m_0}{\tilde{r}_i} + \sum_{i=1}^N \frac{k^2 m_i m_0}{r_i} \right) - \sum_{i=1}^N \frac{k^2 m_i}{r_i} - \sum_{i=1}^N \sum_{j=i+1}^N \frac{k^2 m_i m_j}{|\mathbf{r}_i - \mathbf{r}_j|} \\ &= \sum_{i=1}^N \left( \frac{\tilde{\mathbf{p}}_i^2}{2\tilde{m}_i} - \frac{k^2 m_i m_0}{\tilde{r}_i} \right) + \sum_{i=1}^N \left( \frac{k^2 m_i m_0}{\tilde{r}_i} - \frac{k^2 m_i m_0}{r_i} \right) - \sum_{i=1}^N \sum_{j=i+1}^N \frac{k^2 m_i m_j}{|\mathbf{r}_i - \mathbf{r}_j|} \\ &= \sum_{i=1}^N \left( \frac{\tilde{\mathbf{p}}_i^2}{2\tilde{m}_i} - \tilde{\mu}_i \frac{\tilde{m}_i m_0}{\tilde{r}_i} \right) + k^2 \sum_{i=1}^N m_i m_0 \left( \frac{1}{\tilde{r}_i} - \frac{1}{r_i} \right) - \sum_{i=1}^N \sum_{j=i+1}^N \frac{k^2 m_i m_j}{|\mathbf{r}_i - \mathbf{r}_j|}. \end{aligned} \quad (282)$$

The relationship

$$k^2 m_i = k^2 \frac{m_i}{\tilde{m}_i} \tilde{m}_i$$

$$\begin{aligned}
&= k^2 \frac{\sigma_i}{\sigma_{i-1}} \tilde{m}_i \\
&= k^2 \frac{\tilde{\mu}_i}{k^2} \tilde{m}_i \\
&= \tilde{\mu}_i \tilde{m}_i,
\end{aligned} \tag{283}$$

is used in the first sum in the righthand-side of (282).

Thus the Hamiltonian in (282) becomes a desirable form for the WH map as

$$H = H_{\text{kep}} + \epsilon H_{\text{int}}, \tag{284}$$

where

$$H_{\text{kep}} = \sum_{i=1}^N \left( \frac{\tilde{\mathbf{p}}_i^2}{2\tilde{m}_i} - \tilde{\mu}_i \frac{\tilde{m}_i m_0}{\tilde{r}_i} \right), \tag{285}$$

$$\epsilon H_{\text{int}} = H_{\text{direct}} + H_{\text{indirect}}, \tag{286}$$

$$H_{\text{direct}} = - \sum_{i=1}^N \sum_{j=i+1}^N \frac{k^2 m_i m_j}{|\mathbf{r}_i - \mathbf{r}_j|}, \tag{287}$$

$$H_{\text{indirect}} = k^2 \sum_{i=1}^N m_i m_0 \left( \frac{1}{\tilde{r}_i} - \frac{1}{r_i} \right). \tag{288}$$

The magnitude of  $H_{\text{direct}}$  is  $O(m^2)$ . The magnitude of  $H_{\text{indirect}}$  is also  $O(m^2)$  because of the difference of close terms  $1/\tilde{r}_i - 1/r_i$ ,  $O(m)$ . Hence the magnitude of  $\epsilon H_{\text{int}}$  becomes  $O(m)$  times smaller than that of the Kepler Hamiltonian,  $H_{\text{kep}}$ .

Note that some numerical inaccuracies can arise from  $H_{\text{indirect}}$  in which a subtraction of two quantities at the same order is performed. Straightforward evaluation of these expressions can be avoided by certain reformulation as used in Encke's method (Battin, 1987).

We can also obtain expressions for the angular momentum by the Jacobi coordinates. See Plummer (1960) for detail.

## Two-body Hamiltonian in the Jacobi coordinates and energy integral

Consider the Hamiltonian of the two-body problem written in the Jacobi coordinates using  $\mu = k^2(m_0 + m_1)$ . From (285) when  $N = 1$ , we can easily obtain

$$H_{2\text{body}} = \frac{\tilde{\mathbf{p}}_1^2}{2\tilde{m}_1} - \tilde{\mu}_1 \frac{\tilde{m}_1 m_0}{\tilde{r}_1}. \tag{289}$$

Using the following relationships

$$\tilde{m}_1 = \frac{\sigma_0}{\sigma_1} m_1 = \frac{m_0 m_1}{m_0 + m_1}, \tag{290}$$

$$\tilde{\mu}_1 = \frac{\sigma_1}{\sigma_0} k^2 = \frac{m_0 + m_1}{m_0 m_1} k^2, \tag{291}$$

$$\tilde{\mathbf{r}}_1 = \mathbf{r}_1, \quad \tilde{\mathbf{v}}_1 = \mathbf{v}_1, \quad \tilde{\mathbf{p}}_1 = \tilde{m}_1 \mathbf{v}_1, \tag{292}$$

we get

$$\begin{aligned}
H_{2\text{body}} &= \frac{m_0 + m_1}{2m_0m_1} \left( \frac{m_0m_1}{m_0 + m_1} \mathbf{v}_1 \right)^2 - \frac{m_0 + m_1}{m_0} k^2 \frac{m_0m_1}{m_0 + m_1} \frac{m_0}{r_1} \\
&= \frac{1}{2} \frac{m_0m_1}{m_0 + m_1} \mathbf{v}_1^2 - \frac{k^2 m_1 m_0}{r_1} \\
&= \frac{m_0m_1}{m_0 + m_1} \left( \frac{\mathbf{v}_1^2}{2} - \frac{\mu}{r_1} \right) \\
&= \tilde{m}_1 \left( \frac{\mathbf{v}_1^2}{2} - \frac{\mu}{r_1} \right), \tag{293}
\end{aligned}$$

with a set of canonical variables  $(\tilde{\mathbf{r}}_1, \tilde{\mathbf{p}}_1) = (\mathbf{r}_1, \tilde{m}_1 \mathbf{v}_1)$ .

The equation (293) indicates that the general two-body Hamiltonian  $H_{2\text{body}}$  is not identical to the usual ‘‘energy integral,’’  $\frac{v^2}{2} - \frac{\mu}{r}$ , by a factor of the reduced mass,  $\tilde{m}_1 = \frac{m_0m_1}{m_0+m_1}$ . When we analyzed the error Hamiltonian  $H_{\text{err}}$  in the previous sections, we have taken that this reduced mass  $\tilde{m}_1 = \frac{m_0m_1}{m_0+m_1}$  as unity for simplicity, and treated

$$H_{2\text{body}} = \frac{v_1^2}{2} - \frac{\mu}{r_1}, \tag{294}$$

with canonical variables  $(\mathbf{r}_1, \mathbf{v}_1)$ ; i.e. usual heliocentric position and velocity. We can normalize the two-body Hamiltonian (293) into the form of (294) through a certain conversion of units.

## Appendix B. Canonical relative (DH) coordinates

Let the coordinates and velocities of planets viewed from barycentric frame as  $\boldsymbol{\rho}_i$  and  $\dot{\boldsymbol{\rho}}_i$ . The relationship between the coordinates and velocities based on heliocentric frame  $\mathbf{r}_i$  and  $\dot{\mathbf{r}}_i$  is

$$\boldsymbol{\rho}_i = \mathbf{r}_i - \frac{\sum_{j=1}^N m_j \mathbf{r}_j}{M + \sum_{j=1}^N m_j}, \quad \dot{\boldsymbol{\rho}}_i = \dot{\mathbf{r}}_i - \frac{\sum_{j=1}^N m_j \dot{\mathbf{r}}_j}{M + \sum_{j=1}^N m_j}, \tag{295}$$

where  $N$  is the number of planets and  $M$  is the central mass. If we denote the position of the central mass by  $\boldsymbol{\rho}_c$ ,

$$\begin{aligned}
\boldsymbol{\rho}_c &= \mathbf{r}_c - \frac{\sum_{j=1}^N m_j \mathbf{r}_j}{M + \sum_{j=1}^N m_j} \\
&= -\frac{\sum_{j=1}^N m_j \mathbf{r}_j}{M + \sum_{j=1}^N m_j}, \tag{296}
\end{aligned}$$

since obviously  $\mathbf{r}_c = \mathbf{0}$  in heliocentric coordinate.

Below, we consider separately the kinetic energy and potential energy of the system.

Total kinetic energy of planets  $T_p$  is

$$T_p = \frac{1}{2} \sum_{j=1}^N m_j \dot{\boldsymbol{\rho}}_j^2$$

$$\begin{aligned}
&= \frac{1}{2} \sum_{j=1}^N m_j \left( \dot{\mathbf{r}}_j - \frac{\sum_{i=1}^N m_i \dot{\mathbf{r}}_i}{M + \sum_{i=1}^N m_i} \right)^2 \\
&= \frac{1}{2} \sum_{j=1}^N m_j \left[ \dot{r}_j^2 - \frac{2}{M + \sum_{i=1}^N m_i} \left\{ \dot{\mathbf{r}}_j \cdot \sum_{i=1}^N m_i \dot{\mathbf{r}}_i \right\} + \frac{\left( \sum_{i=1}^N m_i \dot{\mathbf{r}}_i \right) \cdot \left( \sum_{i=1}^N m_i \dot{\mathbf{r}}_i \right)}{\left( M + \sum_{i=1}^N m_i \right)^2} \right].
\end{aligned} \tag{297}$$

The kinetic energy of the central mass  $T_c$  is

$$\begin{aligned}
T_c &= \frac{M}{2} \dot{\boldsymbol{\rho}}_c^2 \\
&= \frac{M}{2} \left( -\frac{\sum_{i=1}^N m_i \dot{\mathbf{r}}_i}{M + \sum_{i=1}^N m_i} \right)^2 \\
&= \frac{M}{2} \frac{\left( \sum_{j=1}^N m_j \dot{\mathbf{r}}_j \right) \cdot \left( \sum_{j=1}^N m_j \dot{\mathbf{r}}_j \right)}{\left( M + \sum_{j=1}^N m_j \right)^2}.
\end{aligned} \tag{298}$$

Hence the total kinetic energy of the system  $T$  becomes

$$\begin{aligned}
T &= T_p + T_c \\
&= \frac{1}{2} \sum_{j=1}^N \left[ m_j \dot{r}_j^2 - m_j \left( \frac{2 \sum_{i=1}^N m_i \dot{\mathbf{r}}_i}{M + \sum_{i=1}^N m_i} \right) \cdot \dot{\mathbf{r}}_j \right. \\
&\quad \left. + \frac{\left( \sum_{i=1}^N m_i \dot{x}_i \right)^2 + \left( \sum_{i=1}^N m_i \dot{y}_i \right)^2 + \left( \sum_{i=1}^N m_i \dot{z}_i \right)^2}{\left( M + \sum_{i=1}^N m_i \right)^2} m_j \right] \\
&\quad + \frac{M}{2} \frac{\left( \sum_{i=1}^N m_i \dot{x}_i \right)^2 + \left( \sum_{i=1}^N m_i \dot{y}_i \right)^2 + \left( \sum_{i=1}^N m_i \dot{z}_i \right)^2}{\left( M + \sum_{i=1}^N m_i \right)^2} \\
&= \frac{1}{2} \sum_{j=1}^N m_j \dot{r}_j^2 - \frac{1}{2} \sum_{j=1}^N m_j \frac{2 \sum_{i=1}^N m_i \dot{\mathbf{r}}_i}{M + \sum_{i=1}^N m_i} \cdot \dot{\mathbf{r}}_j \\
&\quad + \frac{M + \sum_{j=1}^N m_j}{\left( M + \sum_{i=1}^N m_i \right)^2} \cdot \frac{1}{2} \left\{ \left( \sum_{i=1}^N m_i \dot{x}_i \right)^2 + \left( \sum_{i=1}^N m_i \dot{y}_i \right)^2 + \left( \sum_{i=1}^N m_i \dot{z}_i \right)^2 \right\}.
\end{aligned} \tag{299}$$

The second term in the right-hand side of the equation (299) becomes

$$\begin{aligned}
&-\frac{1}{2} \sum_{j=1}^N m_j \underbrace{\left( \frac{2 \sum_{i=1}^N m_i \dot{\mathbf{r}}_i}{M + \sum_{i=1}^N m_i} \right)}_{\text{independent of } j} \cdot \dot{\mathbf{r}}_j = -\frac{1}{2} \left( \frac{2 \sum_{i=1}^N m_i \dot{\mathbf{r}}_i}{M + \sum_{i=1}^N m_i} \right) \sum_{j=1}^N m_j \dot{\mathbf{r}}_j \\
&= -\frac{1}{M + \sum_{i=1}^N m_i} \left( \sum_{i=1}^N m_i \dot{\mathbf{r}}_i \right) \cdot \left( \sum_{j=1}^N m_j \dot{\mathbf{r}}_j \right) \\
&= -\frac{1}{M + \sum_{i=1}^N m_i} \left[ \left( \sum_{i=1}^N m_i \dot{x}_i \right)^2 + \left( \sum_{i=1}^N m_i \dot{y}_i \right)^2 + \left( \sum_{i=1}^N m_i \dot{z}_i \right)^2 \right],
\end{aligned} \tag{300}$$

which ends up with the final form of the total kinetic energy  $T$  as

$$\begin{aligned}
T &= T_p + T_c \\
&= \frac{1}{2} \sum_{j=1}^N m_j \dot{\mathbf{r}}_j^2 - \frac{\left(\sum_{i=1}^N m_i \dot{x}_i\right)^2 + \left(\sum_{i=1}^N m_i \dot{y}_i\right)^2 + \left(\sum_{i=1}^N m_i \dot{z}_i\right)^2}{M + \sum_{i=1}^N m_i} \\
&\quad + \frac{1}{2} \frac{\left(\sum_{i=1}^N m_i \dot{x}_i\right)^2 + \left(\sum_{i=1}^N m_i \dot{y}_i\right)^2 + \left(\sum_{i=1}^N m_i \dot{z}_i\right)^2}{M + \sum_{i=1}^N m_i} \\
&= \frac{1}{2} \sum_{j=1}^N m_j \dot{\mathbf{r}}_j^2 - \frac{1}{2} \frac{\left(\sum_{i=1}^N m_i \dot{x}_i\right)^2 + \left(\sum_{i=1}^N m_i \dot{y}_i\right)^2 + \left(\sum_{i=1}^N m_i \dot{z}_i\right)^2}{M + \sum_{i=1}^N m_i}. \tag{301}
\end{aligned}$$

Thus we can express the total kinetic energy  $T$  only by the heliocentric velocities,  $\dot{\mathbf{r}}_i$ .

If we consider  $\mathbf{r}$  as a canonical coordinate, the canonical conjugate momenta  $\mathbf{p}$  to  $\mathbf{r}$  are derived from Lagrangian

$$L(\mathbf{r}, \dot{\mathbf{r}}) = T(\dot{\mathbf{r}}) - V(\mathbf{r}), \tag{302}$$

where  $T(\dot{\mathbf{r}})$  is kinetic energy and  $V(\mathbf{r})$  is potential energy.

If we define a temporary coordinate  $\mathbf{r}^*$  as

$$\mathbf{r}^* \equiv \frac{1}{M + \sum_{i=1}^N m_i} \sum_{j=1}^N m_j \mathbf{r}_j, \tag{303}$$

then the kinetic energy  $T(\dot{\mathbf{r}})$  is expressed as

$$T(\mathbf{r}) = \frac{1}{2} \sum_{j=1}^N m_j \mathbf{r}_j^2 - \frac{M + \sum_{i=1}^N m_i}{2} \mathbf{r}^{*2}. \tag{304}$$

Hence the canonical momenta  $\mathbf{p}$  become

$$\begin{aligned}
\mathbf{p}_i &\equiv \frac{\partial L}{\partial \dot{\mathbf{r}}_i} \\
&= \frac{\partial}{\partial \dot{\mathbf{r}}_i} (T(\dot{\mathbf{r}}) - V(\mathbf{r}_i)) \\
&= \frac{\partial T}{\partial \dot{\mathbf{r}}_i} \\
&= m_i \dot{\mathbf{r}}_i - \frac{M + \sum_{j=1}^N m_j}{2} 2\dot{\mathbf{r}}^* \cdot \frac{\partial}{\partial \dot{\mathbf{r}}_i} \left( \frac{1}{M + \sum_{j=1}^N m_j} \sum_{j=1}^N m_j \dot{\mathbf{r}}_j \right) \\
&= m_i \dot{\mathbf{r}}_i - \left( M + \sum_{j=1}^N m_j \right) \dot{\mathbf{r}}_i^* \cdot \frac{1}{M + \sum_{j=1}^N m_j} m_i \\
&= m_i (\dot{\mathbf{r}}_i - \dot{\mathbf{r}}_i^*) \\
&= m_i \left( \dot{\mathbf{r}}_i - \frac{1}{M + \sum_{j=1}^N m_j} \sum_{j=1}^N m_j \dot{\mathbf{r}}_j \right). \tag{305}
\end{aligned}$$

The canonical momenta  $\mathbf{p}_i$  in (305) are equivalent to those of what are used in so-called “democratic heliocentric” or “mixed-center” coordinate, which are

$$\mathbf{P}_i \equiv \mathbf{p}_i^{\text{inert}} - \frac{m_i}{M_{\text{total}}} \sum_{j=0}^N \mathbf{p}_j^{\text{inert}}, \tag{306}$$



$$M_{\text{total}} \equiv M + \sum_{i=1}^N m_i, \quad (307)$$

where  $\mathbf{p}_i^{\text{inert}}$  denotes momenta reckoned from a certain fixed point in the inertial frame (for example, barycenter, i.e. essentially the same as  $m_i \boldsymbol{\rho}_i$  in (295)). We now show that the momenta in (305) and momenta in (306) are rigorously equivalent.

Since  $\mathbf{r}$  are the heliocentric coordinate,

$$\dot{\mathbf{r}}_i = \dot{\mathbf{q}}_i - \dot{\mathbf{q}}_0 = \frac{\mathbf{p}_i^{\text{inert}}}{m_i} - \frac{\mathbf{p}_0^{\text{inert}}}{m_0}, \quad (308)$$

where we define  $\mathbf{q}_i$  as the coordinate reckoned from certain fixed point in the inertial frame (this is equivalent to  $\boldsymbol{\rho}_i$  in (295)). Then,  $\mathbf{r}^*$  becomes by (303) as

$$\dot{\mathbf{r}}^* = \frac{1}{M_{\text{total}}} \sum_{j=1}^N m_j \dot{\mathbf{r}}_j = \frac{1}{M_{\text{total}}} \sum_{j=1}^N m_j \left( \frac{\mathbf{p}_j^{\text{inert}}}{m_j} - \frac{\mathbf{p}_0^{\text{inert}}}{m_0} \right). \quad (309)$$

This leads to the expression of  $\mathbf{p}_i$  in (305) as

$$\begin{aligned} \mathbf{p}_i &= m_i \dot{\mathbf{r}}_i - m_i \dot{\mathbf{r}}_i^* \\ &= m_i \left( \frac{\mathbf{p}_i^{\text{inert}}}{m_i} - \frac{\mathbf{p}_0^{\text{inert}}}{m_0} \right) - m_i \frac{1}{M_{\text{total}}} \sum_{j=1}^N m_j \left( \frac{\mathbf{p}_j^{\text{inert}}}{m_j} - \frac{\mathbf{p}_0^{\text{inert}}}{m_0} \right) \\ &= \mathbf{p}_i^{\text{inert}} - \frac{m_i}{m_0} \mathbf{p}_0^{\text{inert}} - \frac{m_i}{M_{\text{total}}} \sum_{j=1}^N m_j \left( \frac{\mathbf{p}_j^{\text{inert}}}{m_j} - \frac{m_j}{m_0} \mathbf{p}_0^{\text{inert}} \right) \\ &= \mathbf{p}_i^{\text{inert}} - \frac{m_i}{M_{\text{total}}} \sum_{j=1}^N \mathbf{p}_j^{\text{inert}} - \frac{m_i}{m_0} \mathbf{p}_0^{\text{inert}} + \frac{m_i}{M_{\text{total}}} \sum_{j=1}^N \frac{m_j}{m_0} \mathbf{p}_0^{\text{inert}} \\ &= \mathbf{p}_i^{\text{inert}} - \frac{m_i}{M_{\text{total}}} \sum_{j=1}^N \mathbf{p}_j^{\text{inert}} + \left( -\frac{m_i}{m_0} + \frac{m_i}{M_{\text{total}}} \sum_{j=1}^N \frac{m_j}{m_0} \right) \mathbf{p}_0^{\text{inert}} \\ &= \mathbf{p}_i^{\text{inert}} - \frac{m_i}{M_{\text{total}}} \sum_{j=1}^N \mathbf{p}_j^{\text{inert}} + \left[ -\frac{m_i}{m_0} \left\{ 1 - \frac{1}{M_{\text{total}}} (M_{\text{total}} - m_0) \right\} \right] \mathbf{p}_0^{\text{inert}} \\ &= \mathbf{p}_i^{\text{inert}} - \frac{m_i}{M_{\text{total}}} \sum_{j=1}^N \mathbf{p}_j^{\text{inert}} - \frac{m_i}{m_0} \left( 1 - \left( 1 - \frac{m_0}{M_{\text{total}}} \right) \right) \mathbf{p}_0^{\text{inert}} \\ &= \mathbf{p}_i^{\text{inert}} - \frac{m_i}{M_{\text{total}}} \sum_{j=1}^N \mathbf{p}_j^{\text{inert}} - \frac{m_i}{M_{\text{total}}} \mathbf{p}_0^{\text{inert}} \\ &= \mathbf{p}_i^{\text{inert}} - \frac{m_i}{M_{\text{total}}} \sum_{j=0}^N \mathbf{p}_j^{\text{inert}}, \end{aligned} \quad (310)$$

which is rigorously equivalent to the momenta used in “democratic heliocentric” (DH) coordinate,  $\mathbf{P}_i$  in (306). The idea of the democratic heliocentric was first advocated by Poincaré and have been described in detail in Charlier (1902) as a name of “*Canonische relative Coordinaten.*” Later, this coordinate was born again to be used in SyMBA in Duncan et al. (1998) as follows.

Below,  $\mathbf{Q}_i$  and  $\mathbf{P}_i$  are canonically conjugate each other.

$$\mathbf{Q}_i = \begin{cases} \mathbf{q}_i - \mathbf{q}_0, & (i = 1, \dots, N) \\ \frac{1}{M_{\text{tot}}} \sum_{j=0}^N m_j \mathbf{q}_j, & (i = 0) \end{cases} \quad (311)$$

$$\mathbf{P}_i = \begin{cases} \mathbf{p}_i - \frac{m_i}{M_{\text{tot}}} \sum_{j=0}^N \mathbf{p}_j, & (i = 1, \dots, N) \\ \sum_{j=0}^N \mathbf{p}_j, & (i = 0) \end{cases} \quad (312)$$

The Hamiltonian described by the DH coordinate is as follows:

$$H = H_{\text{kep}} + H_{\text{sun}} + H_{\text{int}}, \quad (313)$$

$$H_{\text{kep}} = \sum_{i=1}^N \left( \frac{|\mathbf{P}_i|^2}{2m_i} - \frac{Gm_i m_0}{|\mathbf{Q}_i|} \right), \quad (314)$$

$$H_{\text{sun}} = \frac{1}{2m_0} \left| \sum_{i=1}^N \mathbf{P}_i \right|^2, \quad (315)$$

$$H_{\text{int}} = - \sum_{i=1}^{N-1} \sum_{j=i+1}^N \frac{Gm_i m_j}{|\mathbf{Q}_i - \mathbf{Q}_j|}. \quad (316)$$

Note that the Hamiltonian is now divided into three parts, not into two parts as in the generic WH map in (141). This is because of the existence of the Sun's kinetic energy  $H_{\text{sun}}$ . The amount of computation does not increase significantly by the additional procedures due to this new division, since the procedure which involves  $H_{\text{sun}}$  is summing up of linear terms of  $\mathbf{P}$ .

## Appendix C. Partial derivatives of Kepler orbital elements

The partial derivatives of true anomaly  $f$  by the Delaunay variables  $L$  and  $G$  end up with

$$\frac{\partial f}{\partial L} = \frac{G^2}{eL^3} \left( \frac{a}{r} + \frac{L^2}{G^2} \right) \sin f, \quad (317)$$

$$\frac{\partial f}{\partial G} = - \frac{G}{eL^2} \left( \frac{a}{r} + \frac{L^2}{G^2} \right) \sin f, \quad (318)$$

from the relationship

$$\frac{\partial f}{\partial e} = \frac{L^2}{G^2} \sin f. \quad (319)$$

However, we are likely to obtain wrong solutions such as

$$\frac{\partial f}{\partial L} = \frac{G^2}{eL^3} \left( \frac{2a}{r} + \frac{L^2}{G^2} \right) \sin f, \quad (320)$$

or

$$\frac{\partial f}{\partial G} = -\frac{G}{eL^2} \left( \frac{2a}{r} + \frac{L^2}{G^2} \right) \sin f, \quad (321)$$

instead of the correct (317) or (318) due to the usual expressions of  $\frac{\partial f}{\partial e}$  in some of the standard celestial mechanics textbooks (e.g. p. 567 in Brouwer and Clemence (1961), p. 349 in Nagasawa (1983), and Eq. (2.104) at p. 39 in Kinoshita (1998)) as

$$\frac{\partial f}{\partial e} = \left( \frac{a}{r} + \frac{L^2}{G^2} \right) \sin f. \quad (322)$$

To avoid such confusion, we must derive  $\frac{\partial f}{\partial L}$  and  $\frac{\partial f}{\partial G}$  through the definition of differential transformation: using Jacobian matrices.  $\frac{\partial f}{\partial L}$  and  $\frac{\partial f}{\partial G}$  are obtained through a differential transformation of variables from Kepler orbital elements to Delaunay elements as

$$(da, de, d\omega, dI, d\Omega, df) \rightarrow (dL, dG, dH, dl, dg, dh) \quad (323)$$

However, the relationship between  $f$  and  $l$  is not explicit because of the existence of Kepler's equation  $u - e \sin u = l$ . We have to calculate the following three conversion matrices

$$(da, de, d\omega, dI, d\Omega, df) \rightarrow (da, de, d\omega, dI, d\Omega, du), \quad (324)$$

$$(da, de, d\omega, dI, d\Omega, du) \rightarrow (da, de, d\omega, dI, d\Omega, dl), \quad (325)$$

$$(da, de, d\omega, dI, d\Omega, dl) \rightarrow (dL, dG, dH, dl, dg, dh), \quad (326)$$

and multiply them to reach our final goal, (323).

As a set of independent variables to describe the Kepler orbital motion, we consider the following four sets:

- Using mean anomaly  $l$  as  $(a, e, \omega, I, \Omega, l)$
- Using true anomaly  $f$  as  $(a, e, \omega, I, \Omega, f)$
- Using eccentric anomaly  $u$  as  $(a, e, \omega, I, \Omega, u)$
- Delaunay canonical variables  $(L, G, H, l, g, h)$

Hence there are  ${}_4P_2 = 12$  differential transformations among them:

$$\begin{aligned} (da, de, d\omega, dI, d\Omega, df) &\rightarrow (da, de, d\omega, dI, d\Omega, du) \\ (da, de, d\omega, dI, d\Omega, df) &\rightarrow (da, de, d\omega, dI, d\Omega, dl) \\ (da, de, d\omega, dI, d\Omega, df) &\rightarrow (dL, dG, dH, dl, dg, dh) \\ (da, de, d\omega, dI, d\Omega, du) &\rightarrow (da, de, d\omega, dI, d\Omega, dl) \\ (da, de, d\omega, dI, d\Omega, du) &\rightarrow (da, de, d\omega, dI, d\Omega, df) \\ (da, de, d\omega, dI, d\Omega, du) &\rightarrow (dL, dG, dH, dl, dg, dh) \\ (da, de, d\omega, dI, d\Omega, dl) &\rightarrow (da, de, d\omega, dI, d\Omega, df) \\ (da, de, d\omega, dI, d\Omega, dl) &\rightarrow (da, de, d\omega, dI, d\Omega, du) \\ (da, de, d\omega, dI, d\Omega, dl) &\rightarrow (dL, dG, dH, dl, dg, dh) \\ (dL, dG, dH, dl, dg, dh) &\rightarrow (da, de, d\omega, dI, d\Omega, dl) \\ (dL, dG, dH, dl, dg, dh) &\rightarrow (da, de, d\omega, dI, d\Omega, du) \\ (dL, dG, dH, dl, dg, dh) &\rightarrow (da, de, d\omega, dI, d\Omega, df) \end{aligned}$$

This section gives the forward transformations such as

$$\begin{aligned}
& (da, de, d\omega, dI, d\Omega, df) \\
& \quad \downarrow \\
& (da, de, d\omega, dI, d\Omega, du) \\
& \quad \downarrow \\
& (da, de, d\omega, dI, d\Omega, dl) \\
& \quad \downarrow \\
& (dL, dG, dH, dl, dg, dh).
\end{aligned}$$

The latter half can be done similarly, and omitted here.

Note that the lines and columns in the Jacobian matrices described here may be transposed from those in usual textbooks. In the following discussion,

$$r = a(1 - e \cos u) = \frac{a(1 - e^2)}{1 + e \cos f}, \quad (327)$$

$$\eta \equiv \sqrt{1 - e^2}. \quad (328)$$

We frequently consult the relationship between eccentric anomaly  $u$  and true anomaly  $f$

$$\sin u = \frac{\eta \sin f}{1 + e \cos f}, \quad \cos u = \frac{e + \cos f}{1 + e \cos f}, \quad (329)$$

$$\sin f = \frac{\eta \sin u}{1 - e \cos u}, \quad \cos f = \frac{\cos u - e}{1 - e \cos u}. \quad (330)$$

### Appendix C. 1 $(da, de, d\omega, dI, d\Omega, df) \rightarrow (da, de, d\omega, dI, d\Omega, du)$

Since the Kepler orbital elements  $a, e, \omega, I, \Omega$  are independent with each other,

$$\begin{aligned}
\frac{\partial a}{\partial e} &= \frac{\partial a}{\partial \omega} = \frac{\partial a}{\partial I} = \frac{\partial a}{\partial \Omega} = 0, & \frac{\partial a}{\partial a} &= 1, \\
\frac{\partial e}{\partial a} &= \frac{\partial e}{\partial \omega} = \frac{\partial e}{\partial I} = \frac{\partial e}{\partial \Omega} = 0, & \frac{\partial e}{\partial e} &= 1, \\
\frac{\partial \omega}{\partial a} &= \frac{\partial \omega}{\partial e} = \frac{\partial \omega}{\partial I} = \frac{\partial \omega}{\partial \Omega} = 0, & \frac{\partial \omega}{\partial \omega} &= 1, \\
\frac{\partial I}{\partial a} &= \frac{\partial I}{\partial e} = \frac{\partial I}{\partial \omega} = \frac{\partial I}{\partial \Omega} = 0, & \frac{\partial I}{\partial I} &= 1, \\
\frac{\partial \Omega}{\partial a} &= \frac{\partial \Omega}{\partial e} = \frac{\partial \Omega}{\partial I} = \frac{\partial \Omega}{\partial \omega} = 0, & \frac{\partial \Omega}{\partial \Omega} &= 1.
\end{aligned} \quad (331)$$

Hence the differential transformation matrix in this case becomes

$$\begin{pmatrix} da \\ de \\ d\omega \\ dI \\ d\Omega \\ df \end{pmatrix} = \frac{\partial(a, e, \omega, I, \Omega, f)}{\partial(a, e, \omega, I, \Omega, u)} \begin{pmatrix} da \\ de \\ d\omega \\ dI \\ d\Omega \\ du \end{pmatrix}$$

$$\begin{aligned}
&= \begin{pmatrix} \frac{\partial a}{\partial a} & \frac{\partial a}{\partial e} & \frac{\partial a}{\partial \omega} & \frac{\partial a}{\partial I} & \frac{\partial a}{\partial \Omega} & \frac{\partial a}{\partial u} \\ \frac{\partial e}{\partial a} & \frac{\partial e}{\partial e} & \frac{\partial e}{\partial \omega} & \frac{\partial e}{\partial I} & \frac{\partial e}{\partial \Omega} & \frac{\partial e}{\partial u} \\ \frac{\partial \omega}{\partial a} & \frac{\partial \omega}{\partial e} & \frac{\partial \omega}{\partial \omega} & \frac{\partial \omega}{\partial I} & \frac{\partial \omega}{\partial \Omega} & \frac{\partial \omega}{\partial u} \\ \frac{\partial I}{\partial a} & \frac{\partial I}{\partial e} & \frac{\partial I}{\partial \omega} & \frac{\partial I}{\partial I} & \frac{\partial I}{\partial \Omega} & \frac{\partial I}{\partial u} \\ \frac{\partial \Omega}{\partial a} & \frac{\partial \Omega}{\partial e} & \frac{\partial \Omega}{\partial \omega} & \frac{\partial \Omega}{\partial I} & \frac{\partial \Omega}{\partial \Omega} & \frac{\partial \Omega}{\partial u} \\ \frac{\partial f}{\partial a} & \frac{\partial f}{\partial e} & \frac{\partial f}{\partial \omega} & \frac{\partial f}{\partial I} & \frac{\partial f}{\partial \Omega} & \frac{\partial f}{\partial u} \end{pmatrix} \begin{pmatrix} da \\ de \\ d\omega \\ dI \\ d\Omega \\ du \end{pmatrix} \\
&= \begin{pmatrix} 1 & & & \mathbf{0} & 0 \\ & 1 & & & 0 \\ & & 1 & & 0 \\ \mathbf{0} & & & 1 & 0 \\ 0 & \frac{\partial f}{\partial e} & 0 & 0 & \frac{\partial f}{\partial u} \end{pmatrix} \begin{pmatrix} da \\ de \\ d\omega \\ dI \\ d\Omega \\ du \end{pmatrix}. \tag{332}
\end{aligned}$$

Only  $\frac{\partial f}{\partial e}$  and  $\frac{\partial f}{\partial u}$  should be taken into account in all the components of (332).  $\frac{\partial f}{\partial e}$  can be obtained as

$$\begin{aligned}
\frac{\partial}{\partial e} \cos f &= -\sin f \frac{\partial f}{\partial e} \\
&= \frac{\partial}{\partial e} \left( (\cos u - e)(1 - c \cos u)^{-1} \right) \\
&= -1 \cdot (1 - e \cos u)^{-1} + (-e + \cos u) \cdot (-1) \cdot (1 - e \cos u)^{-2} (-\cos u) \\
&= \frac{-1}{1 - e \cos u} + \frac{-e + \cos u}{(1 - e \cos u)^2} \cos u \\
&= \frac{1}{(1 - e \cos u)^2} [-1 + e \cos u + (-e + \cos u) \cos u] \\
&= \frac{1}{(1 - e \cos u)^2} (\cos^2 u - 1) \\
&= \frac{-\sin^2 u}{(1 - e \cos u)^2} \\
&= -\left( \frac{\sin u}{1 - e \cos u} \right)^2 \\
&= -\left( \frac{\sin f}{\eta} \right)^2 \quad (\because (329)) \tag{333}
\end{aligned}$$

$$\therefore \frac{\partial f}{\partial e} = \left( \frac{1}{-\sin f} \right) \left( -\frac{\sin^2 f}{\eta^2} \right) = \frac{1}{\eta^2} \sin f = \frac{L^2}{G^2} \sin f \tag{334}$$

Similarly,  $\frac{\partial f}{\partial u}$  is obtained as

$$\begin{aligned}
\frac{\partial}{\partial u} \cos f &= -\sin f \frac{\partial f}{\partial u} \\
&= \frac{\partial}{\partial u} \left( (\cos u - e)(1 - c \cos u)^{-1} \right) \\
&= -\sin u (1 - e \cos u)^{-1} + (-e + \cos u) \cdot (-1) \cdot (1 - e \cos u)^{-2} e \sin u \\
&= \frac{-\sin u}{1 - e \cos u} - \frac{-e + \cos u}{(1 - e \cos u)^2} e \sin u
\end{aligned}$$

$$\begin{aligned}
&= \frac{1}{(1 - e \cos u)^2} [-\sin u(1 - e \cos u) - e \sin u(-e + \cos u)] \\
&= \frac{\sin u}{(1 - e \cos u)^2} (1 - e^2) \\
&= \frac{\eta^2 \sin^2 u}{(1 - e \cos u)^2} \left( -\frac{1}{\sin u} \right) \\
&= -\frac{\sin^2 f}{\sin u} \quad (\because (329)) \tag{335}
\end{aligned}$$

$$\therefore \frac{\partial f}{\partial u} = \left( -\frac{1}{\sin f} \right) \left( -\frac{\sin^2 f}{\sin u} \right) = \frac{\eta \sin u}{1 - e \cos u} \frac{1}{\sin u} = \frac{a\eta}{r}. \quad (\because (327)) \tag{336}$$

Therefore (332) becomes

$$\begin{aligned}
\begin{pmatrix} da \\ de \\ d\omega \\ dI \\ d\Omega \\ df \end{pmatrix} &= \frac{\partial(a, e, \omega, I, \Omega, f)}{\partial(a, e, \omega, I, \Omega, u)} \begin{pmatrix} da \\ de \\ d\omega \\ dI \\ d\Omega \\ du \end{pmatrix} \\
&= \begin{pmatrix} 1 & & & & \mathbf{0} & 0 \\ & 1 & & & & 0 \\ & & 1 & & & 0 \\ & & & 1 & & 0 \\ \mathbf{0} & & & & 1 & 0 \\ 0 & \frac{\partial f}{\partial e} & 0 & 0 & 0 & \frac{\partial f}{\partial u} \end{pmatrix} \begin{pmatrix} da \\ de \\ d\omega \\ dI \\ d\Omega \\ du \end{pmatrix} \\
&= \begin{pmatrix} 1 & & & & \mathbf{0} & 0 \\ & 1 & & & & 0 \\ & & 1 & & & 0 \\ & & & 1 & & 0 \\ \mathbf{0} & & & & 1 & 0 \\ 0 & \frac{L^2}{G^2} \sin f & 0 & 0 & 0 & \frac{a\eta}{r} \end{pmatrix} \begin{pmatrix} da \\ de \\ d\omega \\ dI \\ d\Omega \\ du \end{pmatrix}. \tag{337}
\end{aligned}$$

Note that at this point

$$\frac{\partial f}{\partial e} = \frac{L^2}{G^2} \sin f, \tag{338}$$

in the final result (337). This expression is due that we consider the true anomaly  $f$  as a function of  $(e, u)$ , not  $(e, l)$  as in (322).

### Appendix C. 2 $(da, de, d\omega, dI, d\Omega, du) \rightarrow (da, de, d\omega, dI, d\Omega, dl)$

When we consider the independence of the mean anomaly  $l$  from any other Kepler orbital elements as

$$\frac{\partial l}{\partial a} = \frac{\partial l}{\partial e} = \frac{\partial l}{\partial \omega} = \frac{\partial l}{\partial I} = \frac{\partial l}{\partial \Omega} = 0, \quad \frac{\partial l}{\partial l} = 1, \tag{339}$$

the differential transformation matrix in this case becomes

$$\begin{aligned}
\begin{pmatrix} da \\ de \\ d\omega \\ dI \\ d\Omega \\ du \end{pmatrix} &= \frac{\partial(a, e, \omega, I, \Omega, u)}{\partial(a, e, \omega, I, \Omega, l)} \begin{pmatrix} da \\ de \\ d\omega \\ dI \\ d\Omega \\ dl \end{pmatrix} \\
&= \begin{pmatrix} \frac{\partial a}{\partial a} & \frac{\partial a}{\partial e} & \frac{\partial a}{\partial \omega} & \frac{\partial a}{\partial I} & \frac{\partial a}{\partial \Omega} & \frac{\partial a}{\partial l} \\ \frac{\partial e}{\partial a} & \frac{\partial e}{\partial e} & \frac{\partial e}{\partial \omega} & \frac{\partial e}{\partial I} & \frac{\partial e}{\partial \Omega} & \frac{\partial e}{\partial l} \\ \frac{\partial \omega}{\partial a} & \frac{\partial \omega}{\partial e} & \frac{\partial \omega}{\partial \omega} & \frac{\partial \omega}{\partial I} & \frac{\partial \omega}{\partial \Omega} & \frac{\partial \omega}{\partial l} \\ \frac{\partial I}{\partial a} & \frac{\partial I}{\partial e} & \frac{\partial I}{\partial \omega} & \frac{\partial I}{\partial I} & \frac{\partial I}{\partial \Omega} & \frac{\partial I}{\partial l} \\ \frac{\partial \Omega}{\partial a} & \frac{\partial \Omega}{\partial e} & \frac{\partial \Omega}{\partial \omega} & \frac{\partial \Omega}{\partial I} & \frac{\partial \Omega}{\partial \Omega} & \frac{\partial \Omega}{\partial l} \\ \frac{\partial u}{\partial a} & \frac{\partial u}{\partial e} & \frac{\partial u}{\partial \omega} & \frac{\partial u}{\partial I} & \frac{\partial u}{\partial \Omega} & \frac{\partial u}{\partial l} \end{pmatrix} \begin{pmatrix} da \\ de \\ d\omega \\ dI \\ d\Omega \\ dl \end{pmatrix} \\
&= \begin{pmatrix} 1 & & & \mathbf{0} & 0 \\ & 1 & & & 0 \\ & & 1 & & 0 \\ & & & 1 & 0 \\ \mathbf{0} & & & & 1 \\ 0 & \frac{\partial u}{\partial e} & 0 & 0 & 0 & \frac{\partial u}{\partial l} \end{pmatrix} \begin{pmatrix} da \\ de \\ d\omega \\ dI \\ d\Omega \\ dl \end{pmatrix}. \tag{340}
\end{aligned}$$

Only  $\frac{\partial u}{\partial e}$  and  $\frac{\partial u}{\partial l}$  should be taken into account in all the components of (340).  $\frac{\partial u}{\partial e}$  can be obtained from the partial derivative of the Kepler's equation

$$u - e \sin u = l, \tag{341}$$

by  $e$

$$\frac{\partial u}{\partial e} - \left( \sin u + e \cos u \frac{\partial u}{\partial e} \right) = \frac{\partial l}{\partial e} = 0. \tag{342}$$

$$\therefore (1 - e \cos u) \frac{\partial u}{\partial e} = \sin u \tag{343}$$

$$\therefore \frac{\partial u}{\partial e} = \frac{\sin u}{1 - e \cos u} = \frac{\sin f}{\eta}. \quad (\because (330)) \tag{344}$$

Similarly,  $\frac{\partial u}{\partial l}$  can be obtained from the partial derivative of the Kepler's equation by  $l$  as

$$\frac{\partial u}{\partial l} - e \cos u \frac{\partial u}{\partial l} = \frac{\partial l}{\partial l} = 1, \tag{345}$$

$$\therefore (1 - e \cos u) \frac{\partial u}{\partial l} = 1, \tag{346}$$

$$\therefore \frac{\partial u}{\partial l} = \frac{1}{1 - e \cos u} = \frac{a}{r}. \tag{347}$$

Therefore the final form of the transformation matrix (340) becomes

$$\begin{aligned}
\begin{pmatrix} da \\ de \\ d\omega \\ dI \\ d\Omega \\ du \end{pmatrix} &= \frac{\partial(a, e, \omega, I, \Omega, u)}{\partial(a, e, \omega, I, \Omega, l)} \begin{pmatrix} da \\ de \\ d\omega \\ dI \\ d\Omega \\ dl \end{pmatrix} \\
&= \begin{pmatrix} 1 & & & \mathbf{0} & 0 \\ & 1 & & & 0 \\ & & 1 & & 0 \\ \mathbf{0} & & & 1 & 0 \\ 0 & \frac{\partial u}{\partial e} & 0 & 0 & \frac{\partial u}{\partial l} \end{pmatrix} \begin{pmatrix} da \\ de \\ d\omega \\ dI \\ d\Omega \\ dl \end{pmatrix} \\
&= \begin{pmatrix} 1 & & & \mathbf{0} & 0 \\ & 1 & & & 0 \\ & & 1 & & 0 \\ \mathbf{0} & & & 1 & 0 \\ 0 & \frac{\sin f}{\eta} & 0 & 0 & \frac{a}{r} \end{pmatrix} \begin{pmatrix} da \\ de \\ d\omega \\ dI \\ d\Omega \\ dl \end{pmatrix}. \tag{348}
\end{aligned}$$

**Appendix C. 3**  $(da, de, d\omega, dI, d\Omega, df) \rightarrow (da, de, d\omega, dI, d\Omega, dl)$

This transformation matrix is obtained as a product of the two matrices

$$\frac{\partial(a, e, \omega, I, \Omega, f)}{\partial(a, e, \omega, I, \Omega, u)}$$

and

$$\frac{\partial(a, e, \omega, I, \Omega, u)}{\partial(a, e, \omega, I, \Omega, l)}$$

as

$$\begin{aligned}
\begin{pmatrix} da \\ de \\ d\omega \\ dI \\ d\Omega \\ df \end{pmatrix} &= \frac{\partial(a, e, \omega, I, \Omega, f)}{\partial(a, e, \omega, I, \Omega, l)} \begin{pmatrix} da \\ de \\ d\omega \\ dI \\ d\Omega \\ dl \end{pmatrix} = \begin{pmatrix} \frac{\partial a}{\partial a} & \frac{\partial a}{\partial e} & \frac{\partial a}{\partial \omega} & \frac{\partial a}{\partial I} & \frac{\partial a}{\partial \Omega} & \frac{\partial a}{\partial l} \\ \frac{\partial e}{\partial a} & \frac{\partial e}{\partial e} & \frac{\partial e}{\partial \omega} & \frac{\partial e}{\partial I} & \frac{\partial e}{\partial \Omega} & \frac{\partial e}{\partial l} \\ \frac{\partial \omega}{\partial a} & \frac{\partial \omega}{\partial e} & \frac{\partial \omega}{\partial \omega} & \frac{\partial \omega}{\partial I} & \frac{\partial \omega}{\partial \Omega} & \frac{\partial \omega}{\partial l} \\ \frac{\partial I}{\partial a} & \frac{\partial I}{\partial e} & \frac{\partial I}{\partial \omega} & \frac{\partial I}{\partial I} & \frac{\partial I}{\partial \Omega} & \frac{\partial I}{\partial l} \\ \frac{\partial \Omega}{\partial a} & \frac{\partial \Omega}{\partial e} & \frac{\partial \Omega}{\partial \omega} & \frac{\partial \Omega}{\partial I} & \frac{\partial \Omega}{\partial \Omega} & \frac{\partial \Omega}{\partial l} \\ \frac{\partial f}{\partial a} & \frac{\partial f}{\partial e} & \frac{\partial f}{\partial \omega} & \frac{\partial f}{\partial I} & \frac{\partial f}{\partial \Omega} & \frac{\partial f}{\partial l} \end{pmatrix} \begin{pmatrix} da \\ de \\ d\omega \\ dI \\ d\Omega \\ dl \end{pmatrix} \\
&= \frac{\partial(a, e, \omega, I, \Omega, f)}{\partial(a, e, \omega, I, \Omega, u)} \frac{\partial(a, e, \omega, I, \Omega, u)}{\partial(a, e, \omega, I, \Omega, l)} \begin{pmatrix} da \\ de \\ d\omega \\ dI \\ d\Omega \\ dl \end{pmatrix}
\end{aligned}$$



$$\begin{aligned}
&= \begin{pmatrix} 1 & & & \mathbf{0} & 0 \\ & 1 & & & 0 \\ & & 1 & & 0 \\ & & & 1 & 0 \\ \mathbf{0} & & & & 1 \\ 0 & \frac{\partial f}{\partial e} & 0 & 0 & 0 \\ & & & & \frac{\partial f}{\partial u} \end{pmatrix} \begin{pmatrix} 1 & & & \mathbf{0} & 0 \\ & 1 & & & 0 \\ & & 1 & & 0 \\ & & & 1 & 0 \\ \mathbf{0} & & & & 1 \\ 0 & \frac{\partial u}{\partial e} & 0 & 0 & 0 \\ & & & & \frac{\partial u}{\partial l} \end{pmatrix} \begin{pmatrix} da \\ de \\ d\omega \\ dI \\ d\Omega \\ dl \end{pmatrix} \\
&= \begin{pmatrix} 1 & & & \mathbf{0} & 0 \\ & 1 & & & 0 \\ & & 1 & & 0 \\ & & & 1 & 0 \\ \mathbf{0} & & & & 1 \\ 0 & \frac{L^2}{G^2} \sin f & 0 & 0 & 0 \\ & & & & \frac{a\eta}{r} \end{pmatrix} \begin{pmatrix} 1 & & & \mathbf{0} & 0 \\ & 1 & & & 0 \\ & & 1 & & 0 \\ & & & 1 & 0 \\ \mathbf{0} & & & & 1 \\ 0 & \frac{\sin f}{\eta} & 0 & 0 & 0 \\ & & & & \frac{a}{r} \end{pmatrix} \begin{pmatrix} da \\ de \\ d\omega \\ dI \\ d\Omega \\ dl \end{pmatrix} \\
&= \begin{pmatrix} 1 & & & \mathbf{0} & 0 \\ & 1 & & & 0 \\ & & 1 & & 0 \\ & & & 1 & 0 \\ \mathbf{0} & & & & 1 \\ 0 & \frac{L^2}{G^2} \sin f + \frac{a\eta}{r} \frac{\sin f}{\eta} & 0 & 0 & 0 \\ & & & & \frac{a\eta}{r} \frac{a}{r} \end{pmatrix} \begin{pmatrix} da \\ de \\ d\omega \\ dI \\ d\Omega \\ dl \end{pmatrix} \\
&= \begin{pmatrix} 1 & & & \mathbf{0} & 0 \\ & 1 & & & 0 \\ & & 1 & & 0 \\ & & & 1 & 0 \\ \mathbf{0} & & & & 1 \\ 0 & \left(\frac{a}{r} + \frac{L^2}{G^2}\right) \sin f & 0 & 0 & 0 \\ & & & & \frac{a^2 \eta}{r^2} \end{pmatrix} \begin{pmatrix} da \\ de \\ d\omega \\ dI \\ d\Omega \\ dl \end{pmatrix}. \tag{349}
\end{aligned}$$

Note that at this point

$$\frac{\partial f}{\partial e} = \left(\frac{a}{r} + \frac{L^2}{G^2}\right) \sin f, \tag{350}$$

in the final result (349). This expression is due that we consider the true anomaly  $f$  as a function of  $(e, l)$ , which is different from the results in (337) where  $f$  is a function of  $(e, u)$ .

#### Appendix C. 4 $(da, de, d\omega, dI, d\Omega, dl) \rightarrow (dL, dG, dH, dl, dg, dh)$

This transformation matrix contains the differential transformation from Kepler orbital elements to Delaunay canonical variables as

$$\begin{pmatrix} da \\ de \\ d\omega \\ dI \\ d\Omega \\ dl \end{pmatrix} = \frac{\partial(a, e, \omega, I, \Omega, l)}{\partial(L, G, H, l, g, h)} \begin{pmatrix} dL \\ dG \\ dH \\ dl \\ dg \\ dh \end{pmatrix} \tag{351}$$

$$= \begin{pmatrix} \frac{\partial a}{\partial L} & \frac{\partial a}{\partial G} & \frac{\partial a}{\partial H} & \frac{\partial a}{\partial l} & \frac{\partial a}{\partial g} & \frac{\partial a}{\partial h} \\ \frac{\partial e}{\partial L} & \frac{\partial e}{\partial G} & \frac{\partial e}{\partial H} & \frac{\partial e}{\partial l} & \frac{\partial e}{\partial g} & \frac{\partial e}{\partial h} \\ \frac{\partial \omega}{\partial L} & \frac{\partial \omega}{\partial G} & \frac{\partial \omega}{\partial H} & \frac{\partial \omega}{\partial l} & \frac{\partial \omega}{\partial g} & \frac{\partial \omega}{\partial h} \\ \frac{\partial I}{\partial L} & \frac{\partial I}{\partial G} & \frac{\partial I}{\partial H} & \frac{\partial I}{\partial l} & \frac{\partial I}{\partial g} & \frac{\partial I}{\partial h} \\ \frac{\partial \Omega}{\partial L} & \frac{\partial \Omega}{\partial G} & \frac{\partial \Omega}{\partial H} & \frac{\partial \Omega}{\partial l} & \frac{\partial \Omega}{\partial g} & \frac{\partial \Omega}{\partial h} \\ \frac{\partial l}{\partial L} & \frac{\partial l}{\partial G} & \frac{\partial l}{\partial H} & \frac{\partial l}{\partial l} & \frac{\partial l}{\partial g} & \frac{\partial l}{\partial h} \end{pmatrix} \begin{pmatrix} dL \\ dG \\ dH \\ dl \\ dg \\ dh \end{pmatrix}. \quad (352)$$

#### Appendix C. 4.1 Partial derivatives of $a$

Representing  $a$  by  $L$  using its definition,

$$a = \frac{L^2}{\mu}. \quad (353)$$

We then know that  $a$  depends only on  $L$ . Hence

$$\frac{\partial a}{\partial L} = \frac{2L}{\mu}, \quad (354)$$

$$\frac{\partial a}{\partial G} = \frac{\partial a}{\partial H} = \frac{\partial a}{\partial l} = \frac{\partial a}{\partial g} = \frac{\partial a}{\partial h} = 0. \quad (355)$$

#### Appendix C. 4.2 Partial derivatives of $e$

Representing  $e$  by Delaunay elements using its definition

$$\frac{G^2}{L^2} = 1 - e^2, \quad (356)$$

$$\therefore e = \sqrt{1 - \frac{G^2}{L^2}}. \quad (357)$$

We then know that  $e$  depends only on  $L$  and  $G$ . Hence

$$\frac{\partial e}{\partial L} = \frac{\partial}{\partial L} \sqrt{1 - \frac{G^2}{L^2}} = \frac{1}{2} \left(1 - \frac{G^2}{L^2}\right)^{-\frac{1}{2}} \frac{2G^2}{L^3} = \frac{G^2}{eL^3}, \quad (358)$$

$$\frac{\partial e}{\partial G} = \frac{\partial}{\partial G} \sqrt{1 - \frac{G^2}{L^2}} = \frac{1}{2} \left(1 - \frac{G^2}{L^2}\right)^{-\frac{1}{2}} \left(-\frac{2G}{L^2}\right) = -\frac{G}{eL^2}, \quad (359)$$

$$\frac{\partial e}{\partial H} = \frac{\partial e}{\partial l} = \frac{\partial e}{\partial g} = \frac{\partial e}{\partial h} = 0. \quad (360)$$

#### Appendix C. 4.3 Partial derivatives of $\omega$

Since the argument of perihelion  $\omega$  is equal to  $g$  by its definition,  $\omega$  is independent from all the other Delaunay variables than  $g$  as

$$\frac{\partial \omega}{\partial L} = \frac{\partial \omega}{\partial G} = \frac{\partial \omega}{\partial H} = \frac{\partial \omega}{\partial l} = \frac{\partial \omega}{\partial h} = 0, \quad \frac{\partial \omega}{\partial g} = 1. \quad (361)$$

#### Appendix C. 4.4 Partial derivatives of $I$

Representing  $I$  by Delaunay elements by its definition

$$\cos I = \frac{H}{G}, \quad (362)$$

which means that  $I$  depends only on  $G$  and  $H$ , which leads to

$$\frac{\partial I}{\partial L} = \frac{\partial I}{\partial l} = \frac{\partial I}{\partial g} = \frac{\partial I}{\partial h} = 0. \quad (363)$$

Partial derivative of (362) by  $G$  gives

$$-\frac{H}{G^2} = -\sin I \frac{\partial I}{\partial G}, \quad (364)$$

$$\therefore \frac{\partial I}{\partial G} = \frac{H}{G^2 \sin I} = \frac{G \cos I}{G^2 \sin I} = \frac{1}{G \tan I}. \quad (365)$$

Similarly, the partial derivative of (362) by  $H$  becomes

$$\frac{1}{G} = -\sin I \frac{\partial I}{\partial H}, \quad (366)$$

$$\therefore \frac{\partial I}{\partial H} = -\frac{1}{G \sin I}. \quad (367)$$

#### Appendix C. 4.5 Partial derivatives of $\Omega$

Since the longitude of ascending node  $\Omega$  is equal to  $h$  by its definition,  $\Omega$  is independent from all the other Delaunay variables than  $h$  as

$$\frac{\partial \Omega}{\partial L} = \frac{\partial \Omega}{\partial G} = \frac{\partial \Omega}{\partial H} = \frac{\partial \Omega}{\partial l} = \frac{\partial \Omega}{\partial g} = 0, \quad \frac{\partial \omega}{\partial h} = 1. \quad (368)$$

#### Appendix C. 4.6 Partial derivatives of $l$

Since the mean anomaly  $l$  is identical to a Delaunay variable  $l$ ,

$$\frac{\partial l}{\partial L} = \frac{\partial l}{\partial G} = \frac{\partial l}{\partial H} = \frac{\partial l}{\partial g} = \frac{\partial l}{\partial h} = 0, \quad \frac{\partial l}{\partial l} = 1. \quad (369)$$

Using results of (354), (355), (358), (359), (360), (361), (363), (365), (367), (368), and (369), the transformation matrix (352) becomes as

$$\begin{aligned} \begin{pmatrix} da \\ de \\ d\omega \\ dI \\ d\Omega \\ dl \end{pmatrix} &= \begin{pmatrix} \frac{\partial a}{\partial L} & 0 & 0 & 0 & 0 & 0 \\ \frac{\partial e}{\partial L} & \frac{\partial e}{\partial G} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & \frac{\partial I}{\partial G} & \frac{\partial H}{\partial G} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} dL \\ dG \\ dH \\ dl \\ dg \\ dh \end{pmatrix} \\ &= \begin{pmatrix} \frac{2L}{eL^3} & 0 & 0 & 0 & 0 & 0 \\ \frac{\mu}{eL^3} & -\frac{G}{eL^2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & \frac{1}{G \tan I} & -\frac{1}{G \sin I} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} dL \\ dG \\ dH \\ dl \\ dg \\ dh \end{pmatrix} \end{aligned} \quad (370)$$



$$\begin{aligned}
& \times \begin{pmatrix} \frac{2L}{eL^3} & 0 & 0 & 0 & 0 & 0 \\ \frac{\mu}{eL^3} & -\frac{G}{eL^2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & \frac{1}{G \tan I} & -\frac{1}{G \sin I} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix} \\
= & \begin{pmatrix} 1 & & & & & \\ & 1 & & & & \\ & & 1 & & & \\ & & & 1 & & \\ \mathbf{0} & & & & 1 & \\ 0 & \left(\frac{a}{r} + \frac{L^2}{G^2}\right) \sin f & 0 & 0 & 0 & \frac{a^2 \eta}{r^2} \end{pmatrix} \begin{pmatrix} \frac{2L}{eL^3} & 0 & 0 & 0 & 0 & 0 \\ \frac{\mu}{eL^3} & -\frac{G}{eL^2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & \frac{1}{G \tan I} & -\frac{1}{G \sin I} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix} \\
= & \begin{pmatrix} \frac{2L}{eL^3} & 0 & 0 & 0 & 0 & 0 \\ \frac{\mu}{eL^3} & -\frac{G}{eL^2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & \frac{1}{G \tan I} & -\frac{1}{G \sin I} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ \frac{G^2}{eL^3} \left(\frac{a}{r} + \frac{L^2}{G^2}\right) \sin f & -\frac{G}{eL^2} \left(\frac{a}{r} + \frac{L^2}{G^2}\right) \sin f & 0 & \frac{a^2 \eta}{r^2} & 0 & 0 \end{pmatrix} \quad (371)
\end{aligned}$$

Hence the final matrix becomes

$$\begin{aligned}
\begin{pmatrix} da \\ de \\ d\omega \\ dI \\ d\Omega \\ df \end{pmatrix} &= \frac{\partial(a, e, \omega, I, \Omega, f)}{\partial(L, G, H, l, g, h)} \begin{pmatrix} dL \\ dG \\ dH \\ dl \\ dg \\ dh \end{pmatrix} \\
&= \begin{pmatrix} \frac{\partial a}{\partial L} & \frac{\partial a}{\partial G} & \frac{\partial a}{\partial H} & \frac{\partial a}{\partial l} & \frac{\partial a}{\partial g} & \frac{\partial a}{\partial h} \\ \frac{\partial e}{\partial L} & \frac{\partial e}{\partial G} & \frac{\partial e}{\partial H} & \frac{\partial e}{\partial l} & \frac{\partial e}{\partial g} & \frac{\partial e}{\partial h} \\ \frac{\partial \omega}{\partial L} & \frac{\partial \omega}{\partial G} & \frac{\partial \omega}{\partial H} & \frac{\partial \omega}{\partial l} & \frac{\partial \omega}{\partial g} & \frac{\partial \omega}{\partial h} \\ \frac{\partial I}{\partial L} & \frac{\partial I}{\partial G} & \frac{\partial I}{\partial H} & \frac{\partial I}{\partial l} & \frac{\partial I}{\partial g} & \frac{\partial I}{\partial h} \\ \frac{\partial \Omega}{\partial L} & \frac{\partial \Omega}{\partial G} & \frac{\partial \Omega}{\partial H} & \frac{\partial \Omega}{\partial l} & \frac{\partial \Omega}{\partial g} & \frac{\partial \Omega}{\partial h} \\ \frac{\partial f}{\partial L} & \frac{\partial f}{\partial G} & \frac{\partial f}{\partial H} & \frac{\partial f}{\partial l} & \frac{\partial f}{\partial g} & \frac{\partial f}{\partial h} \end{pmatrix} \begin{pmatrix} dL \\ dG \\ dH \\ dl \\ dg \\ dh \end{pmatrix} \\
&= \begin{pmatrix} \frac{2L}{eL^3} & 0 & 0 & 0 & 0 & 0 \\ \frac{\mu}{eL^3} & -\frac{G}{eL^2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & \frac{1}{G \tan I} & -\frac{1}{G \sin I} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ \frac{G^2}{eL^3} \left(\frac{a}{r} + \frac{L^2}{G^2}\right) \sin f & -\frac{G}{eL^2} \left(\frac{a}{r} + \frac{L^2}{G^2}\right) \sin f & 0 & \frac{a^2 \eta}{r^2} & 0 & 0 \end{pmatrix} \begin{pmatrix} dL \\ dG \\ dH \\ dl \\ dg \\ dh \end{pmatrix}. \quad (372)
\end{aligned}$$

Thus we have reached the conclusive partial derivatives of (317) and (318).

**Appendix C. 6**  $(da, de, d\omega, dI, d\Omega, du) \rightarrow (dL, dG, dH, dl, dg, dh)$

This transformation matrix is obtained as a product of the two matrices of

$$\frac{\partial(a, e, \omega, I, \Omega, u)}{\partial(a, e, \omega, I, \Omega, l)}$$

and

$$\frac{\partial(a, e, \omega, I, \Omega, l)}{\partial(L, G, H, l, g, h)}$$

as

$$\begin{aligned} \frac{\partial(a, e, \omega, I, \Omega, u)}{\partial(L, G, H, l, g, h)} &= \frac{\partial(a, e, \omega, I, \Omega, u)}{\partial(a, e, \omega, I, \Omega, l)} \frac{\partial(a, e, \omega, I, \Omega, l)}{\partial(L, G, H, l, g, h)} \\ &= \begin{pmatrix} \frac{\partial a}{\partial a} & \frac{\partial a}{\partial e} & \frac{\partial a}{\partial \omega} & \frac{\partial a}{\partial I} & \frac{\partial a}{\partial \Omega} & \frac{\partial a}{\partial l} \\ \frac{\partial e}{\partial a} & \frac{\partial e}{\partial e} & \frac{\partial e}{\partial \omega} & \frac{\partial e}{\partial I} & \frac{\partial e}{\partial \Omega} & \frac{\partial e}{\partial l} \\ \frac{\partial \omega}{\partial a} & \frac{\partial \omega}{\partial e} & \frac{\partial \omega}{\partial \omega} & \frac{\partial \omega}{\partial I} & \frac{\partial \omega}{\partial \Omega} & \frac{\partial \omega}{\partial l} \\ \frac{\partial I}{\partial a} & \frac{\partial I}{\partial e} & \frac{\partial I}{\partial \omega} & \frac{\partial I}{\partial I} & \frac{\partial I}{\partial \Omega} & \frac{\partial I}{\partial l} \\ \frac{\partial \Omega}{\partial a} & \frac{\partial \Omega}{\partial e} & \frac{\partial \Omega}{\partial \omega} & \frac{\partial \Omega}{\partial I} & \frac{\partial \Omega}{\partial \Omega} & \frac{\partial \Omega}{\partial l} \\ \frac{\partial u}{\partial a} & \frac{\partial u}{\partial e} & \frac{\partial u}{\partial \omega} & \frac{\partial u}{\partial I} & \frac{\partial u}{\partial \Omega} & \frac{\partial u}{\partial l} \end{pmatrix} \begin{pmatrix} \frac{\partial a}{\partial L} & \frac{\partial a}{\partial G} & \frac{\partial a}{\partial H} & \frac{\partial a}{\partial l} & \frac{\partial a}{\partial g} & \frac{\partial a}{\partial h} \\ \frac{\partial e}{\partial L} & \frac{\partial e}{\partial G} & \frac{\partial e}{\partial H} & \frac{\partial e}{\partial l} & \frac{\partial e}{\partial g} & \frac{\partial e}{\partial h} \\ \frac{\partial \omega}{\partial L} & \frac{\partial \omega}{\partial G} & \frac{\partial \omega}{\partial H} & \frac{\partial \omega}{\partial l} & \frac{\partial \omega}{\partial g} & \frac{\partial \omega}{\partial h} \\ \frac{\partial I}{\partial L} & \frac{\partial I}{\partial G} & \frac{\partial I}{\partial H} & \frac{\partial I}{\partial l} & \frac{\partial I}{\partial g} & \frac{\partial I}{\partial h} \\ \frac{\partial \Omega}{\partial L} & \frac{\partial \Omega}{\partial G} & \frac{\partial \Omega}{\partial H} & \frac{\partial \Omega}{\partial l} & \frac{\partial \Omega}{\partial g} & \frac{\partial \Omega}{\partial h} \\ \frac{\partial l}{\partial L} & \frac{\partial l}{\partial G} & \frac{\partial l}{\partial H} & \frac{\partial l}{\partial l} & \frac{\partial l}{\partial g} & \frac{\partial l}{\partial h} \end{pmatrix} \\ &= \begin{pmatrix} 1 & & & \mathbf{0} & & \\ & 1 & & & & \\ & & 1 & & & \\ \mathbf{0} & & & 1 & & \\ 0 & \frac{\partial u}{\partial e} & 0 & 0 & 0 & \frac{\partial u}{\partial l} \end{pmatrix} \begin{pmatrix} \frac{\partial a}{\partial L} & 0 & 0 & 0 & 0 & 0 \\ \frac{\partial e}{\partial L} & \frac{\partial e}{\partial G} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & \frac{\partial I}{\partial G} & \frac{\partial H}{\partial G} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix} \\ &= \begin{pmatrix} 1 & & & \mathbf{0} & & \\ & 1 & & & & \\ & & 1 & & & \\ \mathbf{0} & & & 1 & & \\ 0 & \frac{\sin f}{\eta} & 0 & 0 & 0 & \frac{a}{r} \end{pmatrix} \begin{pmatrix} \frac{2L}{eL^3} & 0 & & 0 & 0 & 0 \\ \frac{\mu}{eL^3} & -\frac{G}{eL^2} & & 0 & 0 & 0 \\ 0 & 0 & & 0 & 0 & 1 \\ 0 & \frac{1}{G \tan I} & -\frac{1}{G \sin I} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix} \\ &= \begin{pmatrix} \frac{2L}{eL^3} & 0 & & 0 & 0 & 0 \\ \frac{\mu}{eL^3} & -\frac{G}{eL^2} & & 0 & 0 & 0 \\ 0 & 0 & & 0 & 0 & 1 \\ 0 & \frac{1}{G \tan I} & -\frac{1}{G \sin I} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ \frac{G^2 \sin f}{eL^3 \eta} & -\frac{G \sin f}{eL^2 \eta} & 0 & \frac{a}{r} & 0 & 0 \end{pmatrix} \\ &= \begin{pmatrix} \frac{2L}{eL^3} & 0 & & 0 & 0 & 0 \\ \frac{\mu}{eL^3} & -\frac{G}{eL^2} & & 0 & 0 & 0 \\ 0 & 0 & & 0 & 1 & 0 \\ 0 & \frac{1}{G \tan I} & -\frac{1}{G \sin I} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ \frac{\eta}{eL} \sin f & -\frac{\sin f}{eL} & 0 & \frac{a}{r} & 0 & 0 \end{pmatrix}. \end{aligned} \tag{373}$$

Thus finally,

$$\begin{aligned}
\begin{pmatrix} da \\ de \\ d\omega \\ dI \\ d\Omega \\ du \end{pmatrix} &= \frac{\partial(a, e, \omega, I, \Omega, u)}{\partial(L, G, H, l, g, h)} \begin{pmatrix} dL \\ dG \\ dH \\ dl \\ dg \\ dh \end{pmatrix} \\
&= \begin{pmatrix} \frac{\partial a}{\partial L} & \frac{\partial a}{\partial G} & \frac{\partial a}{\partial H} & \frac{\partial a}{\partial l} & \frac{\partial a}{\partial g} & \frac{\partial a}{\partial h} \\ \frac{\partial e}{\partial L} & \frac{\partial e}{\partial G} & \frac{\partial e}{\partial H} & \frac{\partial e}{\partial l} & \frac{\partial e}{\partial g} & \frac{\partial e}{\partial h} \\ \frac{\partial \omega}{\partial L} & \frac{\partial \omega}{\partial G} & \frac{\partial \omega}{\partial H} & \frac{\partial \omega}{\partial l} & \frac{\partial \omega}{\partial g} & \frac{\partial \omega}{\partial h} \\ \frac{\partial I}{\partial L} & \frac{\partial I}{\partial G} & \frac{\partial I}{\partial H} & \frac{\partial I}{\partial l} & \frac{\partial I}{\partial g} & \frac{\partial I}{\partial h} \\ \frac{\partial \Omega}{\partial L} & \frac{\partial \Omega}{\partial G} & \frac{\partial \Omega}{\partial H} & \frac{\partial \Omega}{\partial l} & \frac{\partial \Omega}{\partial g} & \frac{\partial \Omega}{\partial h} \\ \frac{\partial u}{\partial L} & \frac{\partial u}{\partial G} & \frac{\partial u}{\partial H} & \frac{\partial u}{\partial l} & \frac{\partial u}{\partial g} & \frac{\partial u}{\partial h} \end{pmatrix} \begin{pmatrix} dL \\ dG \\ dH \\ dl \\ dg \\ dh \end{pmatrix} \\
&= \begin{pmatrix} \frac{2L}{\mu} & 0 & 0 & 0 & 0 & 0 \\ \frac{G^2}{eL^3} & -\frac{G}{eL^2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & \frac{1}{G \tan I} & -\frac{1}{G \sin I} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ \frac{\eta}{eL} \sin f & -\frac{\sin f}{eL} & 0 & \frac{a}{r} & 0 & 0 \end{pmatrix} \begin{pmatrix} dL \\ dG \\ dH \\ dl \\ dg \\ dh \end{pmatrix}. \tag{374}
\end{aligned}$$

Now the forward six transformations in

$$(da, de, d\omega, dI, d\Omega, df) \rightarrow (dL, dG, dH, dl, dg, dh)$$

have all been completed.

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