

# Lie-series for orbital elements: II. The spatial case

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Received: 24 April 2014 / Revised: 21 July 2015 / Accepted: 10 September 2015 /  
Published online: 26 September 2015  
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**Abstract** If one has to attain high accuracy over long timescales during the numerical computation of the  $N$ -body problem, the method called Lie-integration is one of the most effective algorithms. In this paper, we present a set of recurrence relations with which the coefficients needed by the Lie-integration of the orbital elements related to the spatial  $N$ -body problem can be derived up to arbitrary order. Similarly to the planar case, these formulae yield identically zero series in the case of no perturbations. In addition, the derivation of the formulae has two stages, analogously to the planar problem. Namely, the formulae are obtained to the first order, and then, higher-order relations are expanded by involving directly the multilinear and fractional properties of the Lie-operator.

**Keywords**  $N$ -body problem · Planetary systems · Numerical methods · Lie-integration

## 1 Introduction

In terms of effectiveness, the method of Lie-integration is one of the most competitive algorithms for numerical computation of gravitational  $N$ -body dynamics. Unlike the “classical” ways for numerical integration, this method computes the Taylor-coefficients of the solution (see Gröbner and Knapp 1967). Hence, the integration itself is relatively straightforward once these coefficients are known. The derivation of the Taylor-coefficients for a particular  $\dot{x}_i = f_i(x_1, \dots, x_N)$  ordinary differential equation is based on the so-called Lie-operator. Recalling the basics of this method, we define this operator as

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**Electronic supplementary material** The online version of this article (doi:[10.1007/s10569-015-9653-0](https://doi.org/10.1007/s10569-015-9653-0)) contains supplementary material, which is available to authorized users.

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$$L := \sum_{i=1}^N f_i \frac{\partial}{\partial x_i}, \quad (1)$$

and by involving this definition, an advancement by  $\Delta t$  of the ordinary differential equation can be written as

$$x_i(t + \Delta t) = \exp(\Delta t L)x_i(t) = \sum_{k=0}^{\infty} \frac{\Delta t^k}{k!} L^k x_i(t). \quad (2)$$

The numerical method called Lie-integration is the finite approximation of the above equation for exponential expansion (up to a certain order which can either be fixed or be adaptively varied, see also Sect. 3.1 in Pál 2010). In order to effectively obtain these coefficients, recurrence formulae can be applied for the Cartesian coordinates of the orbiting bodies which are directly bootstrapped with the initial conditions. Such formulae are known for the gravitational  $N$ -body problem (Hanslmeier and Dvorak 1984; Pál and Süli 2007). A similar kind of relation has been obtained for the restricted three-body problem (Delva 1984), and relativistic and non-gravitational effects (such as Yarkovsky force) can be included as well (Bancelin et al. 2012). In addition, semi-analytic calculations can also be performed to obtain parametric derivatives of observables with respect to orbital elements (Pál 2010).

In this paper, we present such recurrence formulae for the orbital elements in the case of spatial gravitational  $N$ -body problem. Recently, the relations for planar orbital elements have been derived (Pál 2014). Therefore, our goal now is to extend these relations to the third dimension by including the orbital elements *related* to the orbital inclination and ascending node. It should be noted, however, that the relations are not obtained for the longitude of ascending node directly, since it is meaningless in the  $i \rightarrow 0$  limit.

In the following section, Sect. 2, we describe the problem itself and the recurrence relations for the Cartesian coordinates and velocities. The discussion of the spatial problem is split into three parts. Section 3 details the angular momentum vector and the related orbital orientation. The next part, Sect. 4, shows how the orbital eccentricity can be treated in the spatial problem. The set of relations is ended with the mean longitude (Sect. 5). In Sect. 6, we demonstrate how higher-order derivatives are obtained. Our conclusions are summarized in Sect. 7.

## 2 The $N$ -body problem

If we consider Cartesian coordinates and velocities, the recurrence relations for the spatial gravitational  $N$ -body problem have the same structure as in the planar case. Similarly to Pál (2014), let us fix one of the bodies (e.g., the Sun in the case of the Solar System) at the center and this body is orbited by  $N$  additional ones, indexed by  $1 \leq i \leq N$ . In total, we deal with  $1 + N$  bodies, having a mass of  $M$  and  $m_i$ , respectively. If we denote the coordinates and velocities of the  $i$ th body by  $(x_i, y_i, z_i)$  and  $(\dot{x}_i, \dot{y}_i, \dot{z}_i)$ , we can define the central and mutual distances  $\rho_i$  and  $\rho_{ij}$  as  $\rho_i^2 = x_i^2 + y_i^2 + z_i^2$  and  $\rho_{ij}^2 = (x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2$ , the inverse cubic distances  $\phi_i = \rho_i^{-3}$  and  $\phi_{ij} = \rho_{ij}^{-3}$  and the standard gravitational parameters  $\mu_i = G(M + m_i)$ . The quantities  $\Lambda_i = x_i \dot{x}_i + y_i \dot{y}_i + z_i \dot{z}_i$  and  $\Lambda_{ij} = (x_i - x_j)(\dot{x}_i - \dot{x}_j) + (y_i - y_j)(\dot{y}_i - \dot{y}_j) + (z_i - z_j)(\dot{z}_i - \dot{z}_j)$  are also employed in the series of recurrence relations. With these quantities, the recurrence relations for the  $x_i$  coordinates and  $\dot{x}_i$  velocities can be written as

$$L^{n+1}x_i = L^n \dot{x}_i, \quad (3)$$

$$\begin{aligned}
 L^{n+1} \dot{x}_i &= -\mu_i \sum_{k=0}^n \binom{n}{k} L^k \phi_i L^{n-k} x_i \\
 &\quad - \sum_{j \neq i} Gm_j \sum_{k=0}^n \binom{n}{k} \left[ L^k \phi_{ij} L^{n-k} (x_i - x_j) + L^k \phi_j L^{n-k} x_j \right], \tag{4}
 \end{aligned}$$

while the relations for  $y_i$  and  $z_i$  also have the same structure. The relations for the reciprocal cubic distances can be computed in a similar manner as it is done in the planar case, for instance, using Eqs. (3)–(6) from Pál (2014). Once the recurrence relations are obtained and evaluated with the appropriate initial conditions, temporal evolution can be computed with the finite approximation of

$$x_i(t + \Delta t) = \exp(\Delta t L) x_i(t) = \sum_{k=0}^{\infty} \frac{(\Delta t)^k}{k!} L^k x_i(t) \approx \sum_{k=0}^{k_{\max}} \frac{(\Delta t)^k}{k!} L^k x_i(t). \tag{5}$$

Here the summation limit  $k_{\max}$  refers to the maximum integration order. Of course, this calculation is performed not only for the  $x_i$  coordinates but for all of the Cartesian coordinates and velocities.

### 3 The angular momentum and the orientation of the orbit

In the following, we detail the computations and relations comprehending the orbital angular momentum and the orientation of the orbit.

#### 3.1 Angular momentum

In the case of the planar problem, the angular momentum is a pseudoscalar since it is the Hodge dual of a skew-symmetric tensor of rank 2. In the spatial case, the angular momentum is still a skew-symmetric tensor of rank 2; hence, it will have a three-component dual in a form of a pseudovector. For the  $i$ th body, let us denote these 3 components by  $C_{xi}$ ,  $C_{yi}$  and  $C_{zi}$ , respectively. These are computed as

$$C_{xi} = y_i \dot{z}_i - z_i \dot{y}_i, \tag{6}$$

$$C_{yi} = z_i \dot{x}_i - x_i \dot{z}_i, \tag{7}$$

$$C_{zi} = x_i \dot{y}_i - y_i \dot{x}_i. \tag{8}$$

The first-order Lie-derivatives of these pseudovector components can similarly be computed like the pseudoscalar angular momentum in the planar case, viz.

$$LC_{xi} = \sum_{j \neq i} Gm_j \hat{\phi}_{ij} S_{ij}^{[x]}, \tag{9}$$

$$LC_{yi} = \sum_{j \neq i} Gm_j \hat{\phi}_{ij} S_{ij}^{[y]}, \tag{10}$$

$$LC_{zi} = \sum_{j \neq i} Gm_j \hat{\phi}_{ij} S_{ij}^{[z]}, \tag{11}$$

where  $S_{ij}^{[x]}$ ,  $S_{ij}^{[y]}$  and  $S_{ij}^{[z]}$  are defined as

$$S_{ij}^{[x]} = y_i z_j - z_i y_j, \tag{12}$$

$$S_{ij}^{[y]} = z_i x_j - x_i z_j, \tag{13}$$

$$S_{ij}^{[z]} = x_i y_j - y_i x_j, \tag{14}$$

and  $\hat{\phi}_{ij} = \phi_{ij} - \phi_j$ . In order to compute the magnitude of the angular momentum vector,  $C_i$ , we can employ two approaches, as well. First, using the fact that  $C_i^2$  is the sum of squares of the pseudovector components  $C_{xi}$ ,  $C_{yi}$  and  $C_{zi}$ , we can write

$$\frac{1}{2}L(C_i^2) = C_i LC_i = C_{xi} LC_{xi} + C_{yi} LC_{yi} + C_{zi} LC_{zi}. \tag{15}$$

The second alternative is to exploit Lagrange’s identity for cross products, namely

$$\frac{1}{2}C_i^2 = \frac{1}{2}\mathbf{C}_i \cdot \mathbf{C}_i = \frac{1}{2}(\mathbf{r}_i \times \dot{\mathbf{r}}_i) \cdot (\mathbf{r}_i \times \dot{\mathbf{r}}_i) = \frac{1}{2}\mathbf{r}_i^2 \dot{\mathbf{r}}_i^2 - \frac{1}{2}(\mathbf{r}_i \cdot \dot{\mathbf{r}}_i)^2 = \frac{1}{2}\rho_i^2 U_i^2 - \frac{1}{2}\Lambda_i^2, \tag{16}$$

where  $U_i^2 = \dot{x}_i^2 + \dot{y}_i^2 + \dot{z}_i^2$ . Here,  $\rho_i^2 U_i^2$  can be written as  $2\mu_i \rho_i - H_i \rho_i^2$  where  $H_i$  is twice the negative specific energy,  $H_i = 2\mu_i / \rho_i - U_i^2$ . Since both  $H_i$  and  $\Lambda_i$  are scalars, the planar and spatial forms of the first Lie-derivatives are going to be the same:

$$LH_i = 2 \sum_{j \neq i} Gm_j \left[ \phi_{ij} \Lambda_i - \hat{\phi}_{ij} \hat{\Lambda}_{ji} \right], \tag{17}$$

$$L\Lambda_i = \left( U_i^2 - \frac{\mu_i}{\rho_i} \right) + \sum_{j \neq i} Gm_j \left[ \hat{\phi}_{ij} R_{ij} - \phi_{ij} \rho_i^2 \right]. \tag{18}$$

Here  $R_{ij} = x_i x_j + y_i y_j + z_i z_j$  and  $\hat{\Lambda}_{ji} = x_j \dot{x}_i + y_j \dot{y}_i + z_j \dot{z}_i$  (see also Pál 2014). Using the relation  $\frac{1}{2}L(\rho_i^2) = \Lambda_i$ , the above two equations and Eq. (16), it can be seen that

$$\frac{1}{2}L(C_i^2) = \sum_{j \neq i} Gm_j \hat{\phi}_{ij} \left[ \rho_i^2 \hat{\Lambda}_{ji} - \Lambda_i R_{ij} \right]. \tag{19}$$

We should emphasize here that although  $|C_{zi}|$  is equal to  $C_i$  in the planar limit<sup>1</sup>, it does not mean that expressions valid in the planar case could automatically be extended into the spatial form *if* such expressions are functions of pseudoscalars. In the calculations presented in Pál (2014), such differences were tacitly ignored; therefore, one should examine the individual terms before applying these in the third dimension. In fact,  $C_i = \sqrt{C_i^2}$  is a scalar (hence Eq. 19 is valid in both the planar and spatial cases), but  $C_{zi}$  is not—despite the validity of Eq. (11) for the angular momentum in the planar case.

### 3.2 The orientation of the orbit

Using the well-known relations for the longitude of the ascending node  $\Omega$  and the inclination  $i$ , one can compute these by knowing the components of the angular momentum pseudovector:

<sup>1</sup> When  $z_i \rightarrow 0$  and  $\dot{z}_i \rightarrow 0$  for all  $1 \leq i \leq N$ .

$$\sin i_i \cos \Omega_i = -\frac{C_{yi}}{C_i}, \tag{20}$$

$$\sin i_i \sin \Omega_i = +\frac{C_{xi}}{C_i}, \tag{21}$$

$$\cos i_i = \frac{C_{zi}}{C_i}. \tag{22}$$

We note that in the case of small inclinations, the longitude of ascending node is not so well constrained, so in order to avoid roundoff errors or parametric singularities, it is easier to use the Lagrangian orbital elements  $\sin i_i \cos \Omega_i$  and  $\sin i_i \sin \Omega_i$  instead of the angles. Due to the simple relations between the Lagrangian orbital elements and the components of the angular momentum pseudovector, it is also sufficient to deal purely with the  $C_{xi}$ ,  $C_{yi}$  and  $C_{zi}$  terms.

### 3.3 Lie-series for fractions

In the above relations for the Lagrangian ascending node and inclination, fractions appear for quantities whose Lie-series are known. Although recurrence relations for such fractions can be computed in two steps (first by computing the denominator’s reciprocal and then by multiplying it using the Leibniz’ product rule with the numerator), it can be performed in a single step. Let us have two quantities,  $A$  and  $B$  for which the relations are known up to the order  $n$ . It can be shown by mathematical induction that the  $n$ th Lie-derivative of  $A/B = AB^{-1}$  can be written as a function of the Lie-derivatives of  $A$ ,  $B$  up to the order  $n$  and  $AB^{-1}$  up to the order  $n - 1$ :

$$L^n(AB^{-1}) = (L^n A)B^{-1} - B^{-1} \sum_{k=1}^n \binom{n}{k} L^{n-k}(AB^{-1})L^k B. \tag{23}$$

Employing this relation reduces the number of auxiliary quantities that would otherwise have to be introduced for the computation of (more complex) recurrence relations.

## 4 Eccentricity and related quantities

In the spatial case, the longitude of pericenter  $\varpi$  is defined as the sum of longitude of ascending node  $\Omega_i$  and the argument of pericenter,  $\omega_i$ , namely  $\varpi_i = \Omega_i + \omega_i$ . This definition yields the continuity of the longitude of pericenter in the planar limit of  $i_i \rightarrow 0$  when both  $\Omega_i$  and  $\omega_i$  are meaningless. Once  $\varpi_i$  is obtained, the Lagrangian orbital elements  $k_i$  and  $h_i$  are defined accordingly, i.e.,

$$\begin{pmatrix} k_i \\ h_i \end{pmatrix} = e_i \begin{pmatrix} \cos \varpi_i \\ \sin \varpi_i \end{pmatrix}. \tag{24}$$

It can also be deduced that if the  $i$ th orbit is rotated around the line of its nodes into the reference plane, then  $\varpi_i$  and hence  $k_i$  and  $h_i$  are not altered. The aforementioned rotation depends only on the components of the angular momentum vector. Hence, we can write the related rotation matrix as the function of the  $C_{xi}$ ,  $C_{yi}$  and  $C_{zi}$  components as

$$\begin{pmatrix} 1 - \frac{C_{xi}^2}{C_i^2 + C_i C_{zi}} & \frac{-C_{xi} C_{yi}}{C_i^2 + C_i C_{zi}} & -\frac{C_{xi}}{C_i} \\ -\frac{C_{xi} C_{yi}}{C_i^2 + C_i C_{zi}} & 1 - \frac{C_{yi}^2}{C_i^2 + C_i C_{zi}} & -\frac{C_{yi}}{C_i} \\ \frac{C_{xi}}{C_i} & \frac{C_{yi}}{C_i} & \frac{C_{zi}}{C_i} \end{pmatrix} \quad (25)$$

For instance, the coordinate  $x_i$  located in the  $i$ th orbital plane is transformed into:

$$x'_i = x_i - \frac{C_{xi}^2}{C_i^2 + C_i C_{zi}} x_i - \frac{C_{xi} C_{yi}}{C_i^2 + C_i C_{zi}} y_i - \frac{C_{xi}}{C_i} z_i. \quad (26)$$

By exploiting the fact that  $C_{xi}x_i + C_{yi}y_i + C_{zi}z_i = 0$ , the above equation can greatly be simplified:

$$x'_i = x_i - \frac{C_{xi} z_i}{C_i + C_{zi}}. \quad (27)$$

The similar structure can be used for the  $y_i$  coordinate, and the velocity components are also transformed similarly since  $C_{xi}\dot{x}_i + C_{yi}\dot{y}_i + C_{zi}\dot{z}_i$  is also 0. Due to the previously noted invariance of the  $k_i$  and  $h_i$  elements, these can be computed as

$$\begin{pmatrix} k_i \\ h_i \end{pmatrix} = \frac{C_i}{\mu_i} \begin{pmatrix} +\dot{y}'_i \\ -\dot{x}'_i \end{pmatrix} - \frac{1}{\rho_i} \begin{pmatrix} x'_i \\ y'_i \end{pmatrix}. \quad (28)$$

If we substitute Eq. 27 (and the similar relations for  $y_i$ ,  $\dot{x}_i$  and  $\dot{y}_i$ ) into the above equation, we get

$$\begin{pmatrix} k_i \\ h_i \end{pmatrix} = \frac{C_i}{\mu_i} \left[ \begin{pmatrix} +\dot{y}_i \\ -\dot{x}_i \end{pmatrix} - \begin{pmatrix} +p_{yi} \\ -p_{xi} \end{pmatrix} \dot{z}_i \right] - \frac{1}{\rho_i} \left[ \begin{pmatrix} x_i \\ y_i \end{pmatrix} - \begin{pmatrix} p_{xi} \\ p_{yi} \end{pmatrix} z_i \right], \quad (29)$$

where we defined

$$\begin{pmatrix} p_{xi} \\ p_{yi} \end{pmatrix} = \frac{1}{C_i + C_{zi}} \begin{pmatrix} C_{xi} \\ C_{yi} \end{pmatrix}. \quad (30)$$

We note that these  $p_{xi}$  and  $p_{yi}$  quantities are also integrals of motion and can be computed purely from the inclination and longitude of ascending node (but not as simple as in Eqs. 20 or 21). Let us also define the quantities  $a_{xi}$ ,  $a_{yi}$ ,  $a_{zi}$  as

$$a_{xi} = \sum_{i \neq j} Gm_j \left[ \hat{\phi}_{ij} x_j - \phi_{ij} x_i \right], \quad (31)$$

$$a_{yi} = \sum_{i \neq j} Gm_j \left[ \hat{\phi}_{ij} y_j - \phi_{ij} y_i \right], \quad (32)$$

$$a_{zi} = \sum_{i \neq j} Gm_j \left[ \hat{\phi}_{ij} z_j - \phi_{ij} z_i \right]. \quad (33)$$

Using the previously introduced variables, we can compute the first-order Lie-derivatives of  $k_i$  and  $h_i$  as

$$Lk_i = + \left[ \frac{LC_i}{\mu_i} \dot{y}_i + \frac{C_i}{\mu_i} a_{yi} \right] - p_y \left[ \frac{LC_i}{\mu_i} \dot{z}_i - \frac{C_i}{\mu_i} a_{zi} \right] - \left[ + \frac{C_i}{\mu_i} Lp_{yi} \dot{z}_i - \frac{z_i}{\rho_i} Lp_{xi} \right], \quad (34)$$

$$Lh_i = - \left[ \frac{LC_i}{\mu_i} \dot{x}_i + \frac{C_i}{\mu_i} a_{xi} \right] + p_x \left[ \frac{LC_i}{\mu_i} \dot{z}_i - \frac{C_i}{\mu_i} a_{zi} \right] - \left[ - \frac{C_i}{\mu_i} Lp_{xi} \dot{z}_i - \frac{z_i}{\rho_i} Lp_{yi} \right]. \quad (35)$$

Here, the first-order derivatives  $Lp_{xi}$  and  $Lp_{yi}$  can be computed as

$$\begin{pmatrix} Lp_{xi} \\ Lp_{yi} \end{pmatrix} = \frac{1}{C_i + C_{zi}} \left[ \begin{pmatrix} LC_{xi} \\ LC_{yi} \end{pmatrix} - (LC_i + LC_{zi}) \begin{pmatrix} p_{xi} \\ p_{yi} \end{pmatrix} \right]. \tag{36}$$

The derivation of the above equations is similar to the steps performed in Pál (2014). The above two equations for  $Lk_i$  and  $Lh_i$  are clearly zero if mutual perturbations are omitted since then  $LC_i, a_{xi}, a_{yi}, a_{zi}, Lp_{xi}$  and  $Lp_{yi}$  are zero.

As an alternative, one can compute the Lie-derivatives of the Laplace–Runge–Lenz vector. In the spatial case, this vector is defined as

$$\mathbf{e}_i = \frac{1}{\mu_i} (\dot{\mathbf{r}}_i \times \mathbf{C}_i) - \frac{\mathbf{r}_i}{\rho_i}, \tag{37}$$

while all of its components,

$$e_{xi} = \frac{1}{\mu_i} (C_{zi} \dot{y}_i - C_{yi} \dot{z}_i) - \frac{x_i}{\rho_i}, \tag{38}$$

$$e_{yi} = \frac{1}{\mu_i} (C_{xi} \dot{z}_i - C_{zi} \dot{x}_i) - \frac{y_i}{\rho_i}, \tag{39}$$

$$e_{zi} = \frac{1}{\mu_i} (C_{yi} \dot{x}_i - C_{xi} \dot{y}_i) - \frac{z_i}{\rho_i} \tag{40}$$

are integrals of motion. The Lie-derivatives of each of these components have the same structure and can be obtained in a similar manner to the planar case. The first-order Lie-derivatives of the  $(e_{xi}, e_{yi}, e_{zi})$  components are

$$Le_{xi} = \frac{1}{\mu_i} [LC_{zi} \dot{y}_i + C_{zi} a_{yi} - LC_{yi} \dot{z}_i - C_{yi} a_{zi}], \tag{41}$$

$$Le_{yi} = \frac{1}{\mu_i} [LC_{xi} \dot{z}_i + C_{xi} a_{zi} - LC_{zi} \dot{x}_i - C_{zi} a_{xi}], \tag{42}$$

$$Le_{zi} = \frac{1}{\mu_i} [LC_{yi} \dot{x}_i + C_{yi} a_{xi} - LC_{xi} \dot{y}_i - C_{xi} a_{yi}]. \tag{43}$$

In a practical implementation, one could choose whether to compute the Lagrangian orbital elements  $k_i, h_i$  or the components of the vector  $\mathbf{e}_i$ . Due to the constraint

$$\mathbf{C}_i \cdot \mathbf{e}_i = C_{xi} e_{xi} + C_{yi} e_{yi} + C_{zi} e_{zi} = 0, \tag{44}$$

these two sets of variables are equivalent. The first-order Lie-derivatives of both  $(k_i, h_i)$  and  $(e_{xi}, e_{yi}, e_{zi})$  are multilinear expressions of terms whose derivatives are known in advance. Therefore, higher-order derivatives can be computed in a straightforward manner: either using Eq. (24) of Pál (2014) or by introducing auxiliary variables and exploit the product rule for differentials.

### 5 Mean longitude

In order to compute the Lie-derivatives of the mean longitude, we can employ two different approaches. First, similarly to Pál (2014), we write a relatively complex equation for it and then take the full derivative. Here we follow an alternative approach. First, let us write

the mean longitude in the form of  $\lambda_i = M_i + \varpi_i$ , where  $M_i$  is the mean anomaly<sup>2</sup> and  $\varpi_i = \arg(k_i, h_i)$  is the longitude of pericenter. Then, take the first-order Lie-derivatives of both and coadd them in the hope that in the circular limit, the sum  $LM_i + L\varpi_i$  would not be meaningless. Finally, we use this first-order derivative in order to obtain the recurrence relations for higher-order Lie-derivatives.

According to Kepler’s equation, the mean anomaly is computed as  $M_i = E_i - e_i \sin E_i$  where the eccentric anomaly is written in the form of

$$E_i = \arg(e_i \cos E_i, e_i \sin E_i). \tag{45}$$

Although  $E_i$  is still meaningless in the  $e_i \rightarrow 0$  limit, the terms  $e_i \cos E_i$  and  $e_i \sin E_i$  can be computed using the basic relations of two-body kinematics even in the circular case:

$$e_i \cos E_i = 1 - \frac{\rho_i}{a_i} = 1 - \frac{\rho_i H_i}{\mu_i}, \tag{46}$$

$$e_i \sin E_i = \frac{\Lambda_i J_i}{C_i}, \tag{47}$$

where  $J_i := \sqrt{1 - e_i^2}$  (similarly to the definition used in Pál 2014). Then, the first-order Lie-derivative of  $M_i$  is going to be

$$\begin{aligned} LM_i &= L \arg(e_i \cos E_i, e_i \sin E_i) - L(e_i \sin E_i) \\ &= \frac{e_i \cos E_i L(e_i \sin E_i) - e_i \sin E_i L(e_i \cos E_i)}{e_i^2} - L(e_i \sin E_i). \end{aligned} \tag{48}$$

After multiplying by  $e_i^2$  and substituting Eqs. (46) and (47), we get

$$e_i^2 LM_i = \left(1 - \frac{\rho_i H_i}{\mu_i}\right) L \left(\frac{\Lambda_i J_i}{C_i}\right) + \frac{\Lambda_i J_i}{C_i} L \left(\frac{\rho_i H_i}{\mu_i}\right) - (1 - J_i^2) L \left(\frac{\Lambda_i J_i}{C_i}\right). \tag{49}$$

The expansion of the above equation yields the form

$$e_i^2 LM_i = \mu_i^2 \frac{J_i^3}{C_i^3} e_i^2 + \frac{J_i^3}{C_i} \left(1 - \frac{\rho_i \mu_i}{C_i^2}\right) L\Lambda_{pi} + \left(1 + \frac{\rho_i \mu_i}{C_i^2}\right) \frac{J_i \Lambda_i C_i}{2\mu_i^2} LH_i. \tag{50}$$

In this expansion, we use the quantity  $L\Lambda_{pi}$  which is defined as follows. Since  $\Lambda_i$  is not an integral of motion, we split  $L\Lambda_i$  into two parts, viz.

$$L\Lambda_i = \left(U_i^2 - \frac{\mu_i}{\rho_i}\right) + \sum_{i \neq j} Gm_j \left[\hat{\phi}_{ij} R_{ij} - \phi_{ij} \rho_i^2\right] = \left(U_i^2 - \frac{\mu_i}{\rho_i}\right) + L\Lambda_{pi} \tag{51}$$

and then define  $L\Lambda_{pi}$  accordingly. Equation (50) for the mean anomaly has three parts. The first one correspond to Kepler’s third law after dividing by  $e_i^2$ . Despite the fact that in the non-perturbed case, the other two parts are zero, in the perturbed case (when  $L\Lambda_{pi} \neq 0$  or  $LH_i \neq 0$ ), the multipliers are only  $\mathcal{O}(e_i)$  functions, not  $\mathcal{O}(e_i^2)$  functions; therefore,  $LM_i$  is meaningless in the  $e_0 \rightarrow 0$  limit.

The first-order Lie-derivative of the mean longitude can only be computed if  $e_i^2 L\varpi_i$  is added to Eq. (50). The derivative of  $\varpi_i$  is computed using the relation

$$e_i^2 L\varpi_i = k_i Lh_i - h_i Lk_i. \tag{52}$$

<sup>2</sup> Note that the symbol  $M$  represents the central mass while the symbols  $M_i$  (with a single index) denote the mean anomalies.



It can be shown that if we add Eq. (52) to the equation related to the mean anomaly (see Eq. 50), all of the  $\mathcal{O}(e_i)$  terms cancel and  $L\lambda_i$  is continuous in the  $e_i \rightarrow 0$  limit. Without going into the details, here we present the results of this computation. Similarly to the planar case,  $L\lambda_i$  is written into two parts: The first part corresponds to Kepler’s third law, while the another term depends only on the mutual perturbations. Namely,

$$\begin{aligned}
 L\lambda_i = & \frac{1}{\mu_i} H_i^{3/2} + A_0 \rho_i^2 \sum_{j \neq i} Gm_j \phi_{ij} + A_A \sum_{j \neq i} Gm_j \hat{\phi}_{ij} (C_{xi}x_j + C_{yi}y_j) + \\
 & + A_Z \sum_{j \neq i} Gm_j \hat{\phi}_{ij} z_j + A_P \sum_{j \neq i} Gm_j \hat{\phi}_{ij} R_{ij} + A_L \sum_{j \neq i} Gm_j \hat{\phi}_{ij} \hat{\Lambda}_{ji} \tag{53}
 \end{aligned}$$

The expressions for  $A_0, A_A, A_Z, A_P$  and  $A_L$  are the following:

$$A_0 = \frac{1}{C_i} \left( \frac{g_i^{-2} - g_i^{-1}}{1 + J_i} + 2J_i \right), \tag{54}$$

$$A_A = \frac{z_i}{(1 + \cos i_i)^2 C_i^2}, \tag{55}$$

$$A_Z = \frac{z_i}{(1 + \cos i_i) C_i}, \tag{56}$$

$$A_P = \frac{1}{C_i} \left( \frac{J_i^2 (g_i - 1)}{1 + J_i} - 2 \right) + \frac{z_i [C_i^2 A_i \dot{z}_i - \mu_i^2 (2g_i^{-1} - J_i^2) z_i]}{C_i^5 (1 + \cos i_i)^2}, \tag{57}$$

$$A_L = \frac{A_i C_i (1 + g_i)}{\mu_i^2 (1 + J_i)} + \frac{z_i [-C_i^4 g_i^2 \dot{z}_i + A_i \mu_i^2 z_i]}{C_i^3 \mu_i^2 (1 + \cos i_i)^2}, \tag{58}$$

where the dimensionless quantity  $g_i$  is defined as  $g_i := \mu_i \rho_i C_i^{-2}$ .

One should note that the quantity  $A_0$  equals to the quantity with the same name used in Eq. (49) of Pál (2014). We should also warn the reader that in the purely planar case, the expansion of  $L\lambda_i$  involved the quantity  $\hat{C}_{ji} := x_j \dot{y}_i - y_j \dot{x}_i$ . Since this quantity behaves as a pseudoscalar in the purely planar case, it has no direct counterpart in the framework of the spatial problem. Hence, in Eq. (53) we express  $L\lambda_i$  as the function of  $\hat{\Lambda}_{ji}$  instead of such pseudoscalar-like quantities. Therefore, the equivalence of Eq. (53) here and Eq. (49) of Pál (2014) is not obvious at the first glance in the limit of  $z \rightarrow 0$  and  $\dot{z} \rightarrow 0$ . Nevertheless, one could verify this equivalence by considering the relation  $\hat{\Lambda}_{ji}^2 + \hat{C}_{ji}^2 = \rho_j^2 U_i^2$  (where  $\hat{C}_{ji}$  cannot even be defined in the spatial case).

We should note that some of the  $A_*$  terms explicitly contain the third coordinate,  $z_i$  and/or its derivative,  $\dot{z}_i$ . Therefore, in a perturbed system, the time derivative of the mean longitude is not a scalar and this is only invariant for a subgroup of the group  $SO(3)$  of proper rotations. This subgroup is the  $SO(2)$  rotations around the  $z \pm$  axis. On the contrary, the expression for the derivative of mean anomaly  $LM_i$  (see Eq. 50) is a function of scalars. Hence,  $LM_i$  is invariant under arbitrary  $SO(3)$  transformations.

### 6 Higher-order derivatives

Higher-order Lie-derivatives can then almost automatically be derived since all of the corresponding expressions contain multilinear, power and fractional terms for which recurrence relations are known. The bilinear relation follows Leibniz’ product rule; for fractions one

can use the derivation presented in Sect. 3.3, while for powers, one can involve Eq. (51) of Pál (2014). In brief, one can conclude that the Lie-derivatives of any rational function can be computed once the Lie-derivatives of the terms appearing in the function are known in advance.

Actually, higher-order relations for the angular momentum based on Eqs. (9)–(11) can be written as

$$L^{n+1}C_{xi} = \sum_{j \neq i} Gm_j \sum_{k=0}^n \binom{n}{k} L^{n-k} \hat{\phi}_{ij} L^k S_{ij}^{[x]}, \tag{59}$$

$$L^{n+1}C_{yi} = \sum_{j \neq i} Gm_j \sum_{k=0}^n \binom{n}{k} L^{n-k} \hat{\phi}_{ij} L^k S_{ij}^{[y]}, \tag{60}$$

$$L^{n+1}C_{zi} = \sum_{j \neq i} Gm_j \sum_{k=0}^n \binom{n}{k} L^{n-k} \hat{\phi}_{ij} L^k S_{ij}^{[z]}, \tag{61}$$

where the corresponding derivatives of  $L^k \hat{\phi}_{ij}$  are known from earlier works (Hanslmeier and Dvorak 1984; Pál and Süli 2007; Pál 2014) while

$$L^n S_{ij}^{[x]} = \sum_{k=0}^n \binom{n}{k} \left( L^{n-k} y_i L^k z_j - L^{n-k} z_i L^k y_j \right), \tag{62}$$

$$L^n S_{ij}^{[y]} = \sum_{k=0}^n \binom{n}{k} \left( L^{n-k} z_i L^k x_j - L^{n-k} x_i L^k z_j \right), \tag{63}$$

$$L^n S_{ij}^{[z]} = \sum_{k=0}^n \binom{n}{k} \left( L^{n-k} x_i L^k y_j - L^{n-k} y_i L^k x_j \right). \tag{64}$$

Higher-order relations for the Lagrangian orbital elements  $k$  and  $h$  are obtained by expanding the bi- and trilinear terms of Eqs. (34) and (35). This expansion has the following substeps:

- First, the fraction  $L^n [(C_i + C_{zi})^{-1}]$  is needed to be computed, using the rule presented in Sect. 3.3. Here, the numerator is 1 (with zero Lie-derivatives), so Eq. (23) can further be simplified. Alternatively, Eq. (51) of Pál (2014) can be used considering the exponent of  $p = -1$ .
- Once  $L^n [(C_i + C_{zi})^{-1}]$  is known,  $L^{n+1} p_{xi}$  and  $L^{n+1} p_{xi}$  are derived using the trilinear Leibniz’ product rule for Eq. 36.
- The higher-order derivatives of the accelerations  $a_{xi}$ ,  $a_{yi}$  and  $a_{zi}$  are obtained using Leibniz’ rule for two multiplicands, following Eqs. (31)–(33).
- Once these three above steps are done, all of the terms are known appearing in Eqs. (34) and (35). Hence, the trilinear rule should be applied.

In a practical implementation, a programmer needs to treat  $[(C_i + C_{zi})^{-1}]$  as a separate variable and store it accordingly in conjunction with its higher-order derivatives. In addition, a trilinear expansion can also be speeded up if a product like  $L^n(ABC)$  is expanded in two bilinear substeps, namely first one compute  $L^n(AB)$  in the usual manner and then  $L^n(ABC)$  is written as

$$L^n(ABC) = \sum_{k=0}^n \binom{n}{k} L^{n-k}(AB)L^k C. \tag{65}$$

This kind of optimization reduces the number of operations from  $\mathcal{O}(n^2)$  to  $\mathcal{O}(n)$ ; however, auxiliary variables and the respective arrays are needed to be introduced.

The higher-order relations for  $L^{n+1}\lambda_i$  can also be considered similarly since the terms appearing in Eq. (53) are bi-, tri- or quadrilinear functions of the terms  $A_x$  and quantities for which the recurrence relations have already been obtained. The terms  $A_0$ ,  $A_A$ ,  $A_Z$ ,  $A_P$  and  $A_L$  are complex expressions; however, these are still *rational functions* of quantities for which the recurrence series are known.

## 7 Summary

This paper completes the recurrence relations for the Lie-derivatives of the osculating orbital elements in the case of the spatial  $N$ -body problem. These relations can be exploited to integrate directly the equations of motions that are parameterized via the orbital elements. Qualitatively, the advantages and disadvantages of this approach are the same what has been concluded for the planar problem. Namely, evolving orbital elements instead of Cartesian components results in larger stepsizes. On the other hand, the complex implementation and the need of more computing power (for the actual evaluation a single step) could yield only marginal benefit. An initial implementation for a demonstration and validation of the formulae presented in this article can be downloaded from our Web page<sup>3</sup> as well as these codes are available upon request. They are also included in the supplement appended to the electronic version of the paper.

Corresponding to the planar case, coordinates and velocities do appear in the recurrence relations but in a form of purely auxiliary quantities. Further studies can therefore focus on the elimination of the need of coordinates. This is particularly interesting in the case of mean longitude where the third direction is preferred. Such derivations might significantly reduce the computing demands as well.

**Acknowledgments** The author would like to thank A. László for his helpful comments about the tensor rank analysis. The author also thanks the anonymous referees for their thorough reviews of the manuscript. The author thanks László Szabados for the careful proofreading. This work has been supported by the Hungarian Academy of Sciences via the Grant LP2012-31. Additional support is received from the Hungarian OTKA Grants K-109276 and K-104607.

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<sup>3</sup> <http://szofi.elte.hu/~apal/astro/orbitlie/>