Fundamentals of Regularization in Celestial Mechanics and Linear Perturbation Theories

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Abstract

What is regularization? Why is it useful for studying planetary systems? Although collisions in evolved planetary systems are rare events, the theory of regularization (i.e. the removal of collision singularities) is an important tool for developing good perturbation theories and efficient numerical algorithms. We give an overview of these techniques.

1 Introduction

Orbital mechanics of extrasolar planetary systems is based on the widely accepted and well founded assumption that the Newtonian law of gravitation is also valid outside our solar system; in fact we postulate its *universal* validity. Hence many of the basic ingredients of exoplanet research are identical with the foundations of classical celestial mechanis: the motion of a point mass under the Newtonian attraction of a central body and a small perturbation. This fundamental topic, called the perturbed *problem of two bodies*, or for short, the *perturbed Kepler problem* is the main interest of this contribution.

It is therefore appropriate to include here this chapter on classical celestial mechanics in order to revisit the perturbed Kepler problem and its solution. Our goal is to recover the classical theory of Kepler motion and to present a simple theory of the perturbed Kepler problem. For classical perturbation theories see, e.g., Brouwer-Clemence (1961). The common tool is *regularization*, a transformation of both space and time variables introduced by Levi-Civita (1920) in the plane and generalized by Kustaanheimo and Stiefel (1965) in space. Historically, regularization was developed for investigating the singularities of Kelper motion and for describing collisions of two point masses as well as for improving the numerical integration of (near-)collision orbits.

In this context, however, a mere side-effect of the above-mentioned regularizations will be exploited: the *linearity* of the transformed differential equations of motion. Thanks to this linearity and by taking advantage of a unified theory of the planar and spatial cases we will be able to present an elegant treatment of the basics of orbital mechanics.

We illustrate the simplicity of handling perturbed linear problems by means of the following simple example. Consider, e.g., the perturbed system

$$\dot{x}(t) + A(t)\,x(t) - b(t) = \varepsilon f(x,t), \quad x : t \in \mathbb{R} \mapsto x(t) \in \mathbb{R}^n, \tag{1}$$

of linear differential equations, where $A(t)$ is a given time-dependent $(n \times n)$-matrix. Equ. (1) may formally be solved to arbitrary order by the series

$$x(t) = x_0(t) + \varepsilon\, x_1(t) + \varepsilon^2\, x_2(t) + \dots\,,$$

where $x_k(t)$ satisfies the linear differential equation

$$\dot{x_k}(t) + A(t)\,x_k(t) = f_{k-1}(t), \quad k = 0, 1, 2, \dots\,. \tag{2}$$

Here $f_{-1}(t) := b(t)$, and $f_0(t), f_1(t), \dots$ are defined as the coefficients of the formal Taylor series of $f(x,t)$ with respect to ε:

$$\sum_{k=0}^{\infty} \varepsilon^k\, f_k(t) = f\big(x_0(t) + \varepsilon\, x_1(t) + \varepsilon^2\, x_2(t) + \dots\,, t\big)\,.$$

Note that the linear differential equations (2) are all of the type of the unperturbed problem $k = 0$; they only differ in their right-hand sides.

We will begin by collecting the well-known classical formulas governing planar elliptic Kepler motion (essentially the three Keplerian laws and some geometry of conic sections). Simple properties of these equations will provide a natural motivation for Levi-Civita's regularization. In Section 3 we will describe in detail the planar regularization procedure and show that the resulting linear system of differential equations is even of a very special form: a harmonic oscillator. Section 4 will present the corresponding spacial regularization, elegantly represented by means of quaternions. In Section 5 we will discuss the linear perturbation theories of Kepler motion as a perturbed harmonic oscillator.

2 Planar Kepler Motion

Consider Kepler motion of a massless particle positioned at $x = \binom{x_1}{x_2} \in \mathbb{R}^2$ around a central body with gravitational parameter μ. For convenience the position of the particle will equivalently be denoted by the complex coordinate $\mathbf{x} = x_1 + i\,x_2 \in \mathbb{C}$ (complex numbers will be denoted by bold face characters). Kepler motion is then governed by the differential equation

$$\ddot{\mathbf{x}} + \mu\,\frac{\mathbf{x}}{r^3} = 0\,, \quad r = |\,\mathbf{x}\,|\,, \tag{3}$$

where dots denote derivatives with respect to time t. The Keplerian orbit of

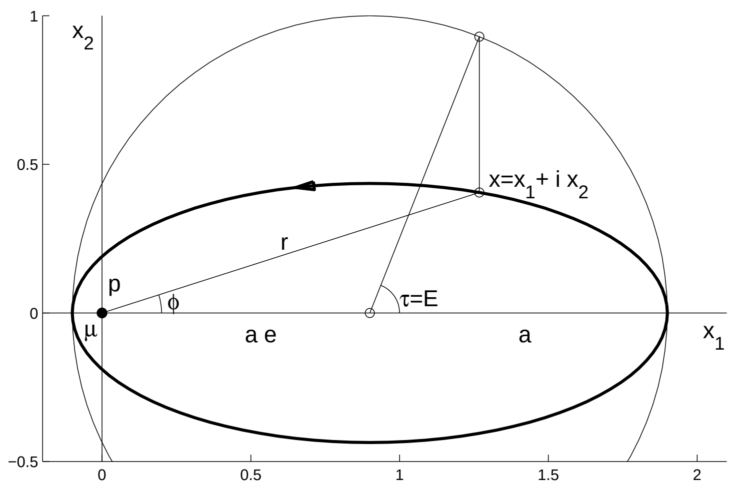

Figure 1: The planar elliptic Kepler motion with eccentricity $e = 0.9$

Figure 1 is standardized such that the apocenter is on the x_1-axis; therefore the orbit is given by merely two *orbital elements,* e.g. the major semi-axis a and the eccentricity e. An important orbital element depending on a and e is the semi-latus rectum $p = a\,(1 - e^2)$. Quantities varying with the moving particle are the radial distance $r = |\,\mathbf{x}\,|$ and the polar angle $\varphi = \arg(\mathbf{x})$ as well as the eccentric anomaly E (see Figure 1), which turns out to be the parameter best suited for completely describing Kepler motion in space and time.

The famous relations describing the orbit are

$$x_1 = a\,(e + \cos E\,)\,, \quad x_2 = a\,\sqrt{1 - e^2} \cdot \sin E\,, \tag{4}$$

which implies

$$r = |\,\mathbf{x}\,| = a\,(1 + e\,\cos E)\,. \tag{5}$$

For detemining the time t (normalized such that a passage through the apocenter is at $t = 0$) we may use the famous *Keplerian equation* and its derivative,

$$t = \sqrt{\frac{a^3}{\mu}} \cdot (E + e\,\sin E)\,, \quad \frac{dt}{dE} = \sqrt{\frac{a}{\mu}} \cdot r\,. \tag{6}$$

Keplerian orbits have a simple representation in polar coordinates,

$$r = \frac{p}{1 - e\,\cos\varphi}\,, \qquad p = a\,(1 - e^2)\,, \tag{7}$$

where the relation between E and φ, precise $\bmod 2\pi$, may be written as

$$\tan(\frac{\varphi}{2}) = \sqrt{\frac{1-e}{1+e}}\,\tan(\frac{E}{2})\,. \tag{8}$$

Finally, we mention the conservation of energy

$$\frac{1}{2}\,|\,\dot{\mathbf{x}}\,|^2 - \frac{\mu}{r} = -h = \text{const}\,, \quad h = \frac{\mu}{2\,a} > 0\,, \tag{9}$$

where the energy constant is denoted by $-h$, such that $h > 0$ corresponds to the elliptic case, and the conservation of angular momentum,

$$|\,x \times \dot{x}\,| = \sqrt{\mu\,p} = \text{const}\,. \tag{10}$$

We now try to exploit properties of these relations in order to find appropriate variables for a simple description of Kepler motion.

(i) Equs. (4) and (6) suggest that E might be a more suitable independent variable than the time t. In generalization of the transformation used by Sundman (1907) we introduce a *fictitious time* τ according to the differential relation

$$dt = \frac{r}{c} \cdot d\tau\,, \quad r = |\,\mathbf{x}\,|\,. \tag{11}$$

With $c = 1\,,\ \tau$ is Sundman's variable, whereas, according to Equs. (6_2) and (9), $c = \sqrt{2\,h}$ introduces the eccentric anomaly $\tau = E$ as the new independent variable.

(ii) Consider the complex position $\mathbf{x} \in \mathbb{C}$, written in terms of E by means of Equ. (4),

$$\mathbf{x} = x_1 + i\,x_2 = a\,\left(e + \cos E + i\,\sqrt{1-e^2}\,\sin E\right)\,.$$

Note that $\mathbf{x} = \mathbf{u}^2 \in \mathbb{C}$ is identically the square of

$$\mathbf{u} = \sqrt{a\,(1+e)}\,\cos(\frac{E}{2}) + i\,\sqrt{a\,(1-e)}\,\sin(\frac{E}{2})\,. \tag{12}$$

This is precisely the conformal mapping between the the parametric $\mathbf{u}$-plane and the physical $\mathbf{x}$-plane used by Levi-Civita: a conformal *squaring*.

3 The Levi-Civita Transformation

In this section we carry out the *three* steps necessary for regularizing the unperturbed planar Kepler problem by Levi-Civita's method. The first two steps exactly follow the suggestions (i) and (ii) discussed above. The third step will merely consist of fixing the energy. In the following, we will therefore subject the equations of motion (3) as well as the energy equation (9_1) to the transformations of the first two steps. Complex notation will be used throughout, i.e. instead of the vector $x = \binom{x_1}{x_2} \in \mathbb{R}^2$ we use the corresponding complex coordinate $\mathbf{x} = x_1 + i\,x_2 \in \mathbb{C}$.

3.1 First step: Slow-motion movie

Instead of the physical time t a new independent variable τ, the fictitious time, is introduced by the differential relation (11); derivatives with respect to τ will be denoted by primes. Therefore the ratio $dt/d\tau$ of two infinitesimal increments is made proportional to the distance r; the movie is run in slow-motion whenever r becomes small. With the differentiation rules

$$\frac{d}{dt} = c\, r^{-1} \frac{d}{d\tau}\,, \qquad \frac{d^2}{dt^2} = c^2 \left(r^{-2} \frac{d^2}{d\tau^2} + (\frac{c'}{c}\, r - r')\, r^{-3} \frac{d}{d\tau} \right)$$

Equs. (3) and (9) are transformed into

$$c^2 \Big(r\, \mathbf{x}'' + (\frac{c'}{c}\, r - r')\, \mathbf{x}' \Big) + \mu\, \mathbf{x} = 0\,, \qquad \frac{1}{2}\, c^2\, r^{-2}\, |\mathbf{x}'|^2 - \frac{\mu}{r} = -h\,. \qquad (13)$$

3.2 Second step: Conformal squaring

This part of Levi-Civita's regularization procedure consists of representing the complex physical coordinate $\mathbf{x}$ as the square $\mathbf{u}^2$ of a complex variable $\mathbf{u} = u_1 + i\, u_2 \in \mathbb{C}$,

$$\mathbf{x} \;=\; \mathbf{u}^2\,, \qquad (14)$$

i.e. the mapping from the parametric plane to the physical plane is chosen as a conformal squaring. Equ. (14) implies

$$r \;=\; |\,\mathbf{x}\,| \;=\; |\,\mathbf{u}\,|^2 \;=\; \mathbf{u}\,\bar{\mathbf{u}}\,, \qquad (15)$$

and differentiation of Equs. (14) and (15) yields

$$\mathbf{x}' = 2\, \mathbf{u}\, \mathbf{u}'\,, \quad \mathbf{x}'' = 2\, \left(\mathbf{u}\, \mathbf{u}'' + \mathbf{u}'^{\,2} \right) \in \mathbb{C}\,, \quad r' = \mathbf{u}'\, \bar{\mathbf{u}} + \bar{\mathbf{u}}'\,. \qquad (16)$$

Substitution of this into Equ. (13_1) and cancelling two equal terms ($2\, r\, \mathbf{u}'^2$ and $2\, \mathbf{u}'\, \bar{\mathbf{u}}\, \mathbf{u}\, \mathbf{u}'$) as well as dividing by $c^2\, \mathbf{u}$ yields

$$2\, r\, \mathbf{u}'' + 2\, \frac{c'}{c}\, r\, \mathbf{u}' + (\, \frac{\mu}{c^2} - 2\, |\, \mathbf{u}'\, |^{\,2}\,)\, \mathbf{u} = 0\,. \qquad (17)$$

Although we have $c' = 0$ in this section, the second term has been retained in view the perturbed Kepler motion to be considered later. Similarly, substitution into the energy equation (13_2) yields

$$2\, c^2\, |\, \mathbf{u}'\, |^{\,2} = \mu - r\, h\,. \qquad (18)$$

3.3 Third step: Fixing the energy

This final regularization step amounts to considering only orbits of the fixed energy $-h$. Then, the nonlinear factor $|\,\mathbf{u}'\,|^{\,2}$ may conveniently be eliminated from the equations (17) and (18). Multiplying the result by c^2/r yields

$$2\,c^2\,\mathbf{u}'' + 2\,c\,c'\,\mathbf{u}' + h\,\mathbf{u} = 0\,, \quad \mathbf{u} \in \mathbb{C}\,. \tag{19}$$

In the unperturbed case $c' = 0$ this reduces to the differential equation

$$\mathbf{u}'' + \omega^2\,\mathbf{u} = 0\,, \quad \mathbf{u} \in \mathbb{C}\,, \quad \omega := c^{-1}\,\sqrt{h/2} \tag{20}$$

of a harmonic oscillator of frequency ω in 2 dimensions. For Sundmun's choice $c = 1$ Equ. (20) simply becomes $2\,\mathbf{u}'' + h\,\mathbf{u} = 0$.

Remark 1. Based on the preceding part of this section we propose an alternate way of deriving the Kepler formulas of Section 2. We depart from the equations of motion (3), possibly together with the energy integral (9) and the angular-momentum integral (10). Next, carrying out the three steps of the Levi-Civita regularization procedure results in Equ. (19). A favourable choice is $c = \sqrt{2\,h} =$ const, resulting in the oscillator equation $\mathbf{u}'' + \frac{1}{4}\,\mathbf{u} = 0$. With no loss of generality (and in an appropriate normalization) we write its general solution as $\mathbf{u} = A\,\cos(\frac{E}{2}) + i\,B\,\sin(\frac{E}{2})$ with $A, B \in \mathbb{R}$.

Now the entire theory of planar Kepler motion may be recovered from elementary calculations and some geometry of conic sections:

- the parametrization (4) and Equ. (5)
- the geometric meaning of E
- the energy integral and Equ. (9_2)
- the time evolution, Kepler's equation, Equ. (6)
- Kepler's third law
- the orbit in polar coordinates, Equ. (7)
- the angular-momentum integral, Equ. (10) .

Remark 2. Obtaining initial values $\mathbf{u}(0) = \sqrt{\mathbf{x}(0)} \in \mathbb{C}$ requires the computation of a complex square root. This can conveniently be accomplished by means of the formula

$$\sqrt{\mathbf{x}} = \frac{\mathbf{x} + |\mathbf{x}|}{\sqrt{2\,(|\mathbf{x}| + \operatorname{Re}\mathbf{x})}}\,, \tag{21}$$

which reflects the observation that the complex vector $\sqrt{\mathbf{x}}$ has the direction of the bisector between $\mathbf{x}$ and the real vector $|\mathbf{x}|$; it holds in the range $-\pi < \arg(\mathbf{x}) < \pi$. The alternative formula

$$\sqrt{\mathbf{x}} = \frac{\mathbf{x} - |\mathbf{x}|}{i\,\sqrt{2\,\,(|\mathbf{x}| - \operatorname{Re}\mathbf{x})}}$$

holds in $0 < \arg(\mathbf{x}) < 2\pi$ and agrees with (21) in the upper half-plane; it therefore provides the analytic continuation of (21) into the sector $\pi \leq \arg(\mathbf{x}) < 2\pi$. Furthermore, it avoids a loss of accuracy near the negative real axis $\mathbf{x} < 0$.

4 Spatial Regularization with Quaternions

In this section we indicate how Levi-Civita's regularization procedure may be generalized to three-dimensional motion. The essential step is to replace the conformal squaring of Section 3 by the Kustaanheimo-Stiefel (KS) transformation. A preliminary version of this transformation using spinor notation was proposed by Kustaanheimo (1964); the full theory was developed in a subsequent joint paper (Kustaanheimo and Stiefel, 1965); the entire topic is extensively discussed in the comprehensive text by Stiefel and Scheifele (1971). The relevant mapping from the 3-sphere onto the 2-sphere was already discovered by Heinz Hopf (1931) and is referred to in topology as the Hopf mapping.

Both the Levi-Civita and the Kustaanheimo-Stiefel regularization share the property of "linearizing" the equations of motion of the two-body problem; both are therefore well suited for developing linear perturbation theories. Quaternion algebra, introduced by W. R. Hamilton (1844), turns out to be the ideal tool for regularizing the three-dimensional Kepler motion, as was observed by M. D. Vivarelli (1983) and J. Vrbik (1994, 1995). It was observed by Waldvogel (2006a, 2006b) that by introducing an unconventional conjugation, the *star conjugation* of quaternions, (see the definition in Equ. (29)

below) the spatial regularization procedure according to Kustaanheimo and Stiefel is in complete formal agreement with Levi-Civita's planar procedure described in Section 3. Here we will repeat or summarize the relevant parts of those papers.

4.1 Basics

Quaternion algebra is a generalization of the algebra of complex numbers obtained by using three independent "imaginary" units i, j, k. As for the single imaginary unit i in the algebra of complex numbers, the rules

$$i^2 = j^2 = k^2 = -1$$

are postulated, together with the non-commutative multiplication rules

$$i\,j = -j\,i = k\,, \quad j\,k = -k\,j = i\,, \quad k\,i = -i\,k = j\,.$$

Given the real numbers $u_l \in \mathbb{R}\,,\ l = 0, 1, 2, 3$, the object

$$\mathbf{u} = u_0 + i\,u_1 + j\,u_2 + k\,u_3 \tag{22}$$

is called a *quaternion* $\mathbf{u} \in \mathbb{U}$, where $\mathbb{U}$ denotes the set of all quaternions (in the remaining sections bold-face characters denote quaternions). The sum $iu_1 + ju_2 + ku_3$ is called the *quaternion part* of $\mathbf{u}$, whereas u_0 is naturally referred to as its real part. The above multiplication rules and vector space addition define the *quaternion algebra.* Multiplication is generally non-commutative; however, any quaternion commutes with a real:

$$c\,\mathbf{u} = \mathbf{u}\,c\,, \quad c \in \mathbb{R}\,,\ \mathbf{u} \in \mathbb{R}\,, \tag{23}$$

and for any three quaternions $\mathbf{u}$, $\mathbf{v}$, $\mathbf{w} \in \mathbb{U}$ the associative law holds:

$$(\mathbf{u}\,\mathbf{v})\,\mathbf{w} = \mathbf{u}\,(\mathbf{v}\,\mathbf{w})\,. \tag{24}$$

The quaternion $\mathbf{u}$ may naturally be associated with the corresponding vector $u = (u_0, u_1, u_2, u_3) \in \mathbb{R}^4$. For later reference we introduce notation for 3-vectors in two important particular cases: $\vec{u} = (u_1, u_2, u_3) \in \mathbb{R}^3$ for the vector associated with the *pure quaternion* $\mathbf{u} = i\,u_1 + j\,u_2 + k\,u_3$, and $\underline{u} = (u_0, u_1, u_2)$ for the vector associated with the quaternion with a vanishing k-component, $\mathbf{u} = u_0 + i\,u_1 + j\,u_2$.

For convenience we also introduce the vector $\vec{\imath} = (i, j, k)$; the quaternion $\mathbf{u}$ may then be written formally as $\mathbf{u} = u_0 + \langle \vec{\imath}, \vec{u} \rangle$, where the notation $\langle \cdot\,, \cdot \rangle$ refers to the dot product of vectors. For the two quaternion products of $\mathbf{u}$ and $\mathbf{v} = v_0 + \langle \vec{\imath}, \vec{v} \rangle$ we then obtain the concise expressions

$$\begin{aligned} \mathbf{u}\,\mathbf{v} &= u_0 v_0 - \langle \vec{u}, \vec{v} \rangle + \langle \vec{\imath},\, u_0\, \vec{v} + v_0\, \vec{u} + \vec{u} \times \vec{v} \rangle \\ \mathbf{v}\,\mathbf{u} &= u_0 v_0 - \langle \vec{u}, \vec{v} \rangle + \langle \vec{\imath},\, u_0\, \vec{v} + v_0\, \vec{u} - \vec{u} \times \vec{v} \rangle \,, \end{aligned} \tag{25}$$

where $\times$ denotes the vector product. Note that the non-commutativity shows only in the sign of the term with the vector product.

The *conjugate* $\bar{\mathbf{u}}$ of the quaternion $\mathbf{u}$ is defined as

$$\bar{\mathbf{u}} = u_0 - i\, u_1 - j\, u_2 - k\, u_3 \,; \tag{26}$$

then the *modulus* $|\mathbf{u}|$ of $\mathbf{u}$ is obtained from

$$|\mathbf{u}\,|^2 = \mathbf{u}\,\bar{\mathbf{u}} = \bar{\mathbf{u}}\,\mathbf{u} = \sum_{l=0}^{3} u_l^2 \,. \tag{27}$$

As transposition of a product of matrices, conjugation of a quaternion product reverses the order of its factors:

$$\overline{\mathbf{u}\,\mathbf{v}} = \bar{\mathbf{v}}\,\bar{\mathbf{u}} \,. \tag{28}$$

4.2 The KS Map in the Language of Quaternions

We first revisit the KS transformation by using quaternion algebra and the unconventional "conjugate" $\mathbf{u}^\star$, referred to as the *star conjugate* of the quaternion $\mathbf{u} = u_0 + i\, u_1 + j\, u_2 + k\, u_3$,

$$\mathbf{u}^\star := u_0 + i\, u_1 + j\, u_2 - k\, u_3 \,, \tag{29}$$

introduced by Waldvogel (2006a). The star conjugate of $\mathbf{u}$ may be expressed in terms of the conventional conjugate $\bar{\mathbf{u}}$ as

$$\mathbf{u}^\star = k\, \bar{\mathbf{u}}\, k^{-1} = -k\, \bar{\mathbf{u}}\, k \,;$$

however, it turns out that the definition (29) leads to a particularly elegant treatment of KS regularization. The following elementary properties are easily verified:

$$\begin{aligned}(\mathbf{u}^\star)^\star &= \mathbf{u}\\ |\,\mathbf{u}^\star|^2 &= |\mathbf{u}|^2\\ (\mathbf{u}\,\mathbf{v})^\star &= \mathbf{v}^\star\,\mathbf{u}^\star\,.\end{aligned} \tag{30}$$

Consider now the mapping

$$\mathbf{u}\in\mathbb{U}\;\longmapsto\;\mathbf{x}=\mathbf{u}\,\mathbf{u}^\star\;. \tag{31}$$

Star conjugation immediately yields $\mathbf{x}^\star = (\mathbf{u}^\star)^\star\,\mathbf{u}^\star = \mathbf{x}$; hence $\mathbf{x}$ is a quaternion of the form $\mathbf{x} = x_0 + i\,x_1 + j\,x_2$ which may be associated with the vector $\underline{x} = (x_0, x_1, x_2) \in \mathbb{R}^3$. From $\mathbf{u} = u_0 + i\,u_1 + j\,u_2 + k\,u_3$ we obtain

$$\begin{aligned}x_0 &= u_0^2 - u_1^2 - u_2^2 + u_3^2\\ x_1 &= 2(u_0\,u_1 - u_2\,u_3)\\ x_2 &= 2(u_0\,u_2 + u_1\,u_3)\;,\end{aligned} \tag{32}$$

which is exactly the KS transformation in its classical form or – up to a permutation of the indices – the Hopf map. Therefore we have

Theorem 1: The KS transformation which maps $u = (u_0, u_1, u_2, u_3) \in \mathbb{R}^4$ to $\underline{x} = (x_0, x_1, x_2) \in \mathbb{R}^3$ is given by the quaternion relation

$$\mathbf{x} = \mathbf{u}\,\mathbf{u}^\star\,,$$

where $\mathbf{u} = u_0 + i\,u_1 + j\,u_2 + k\,u_3\,,\ \mathbf{x} = x_0 + i\,x_1 + j\,x_2$. □

Corollary 1: The norms of the vectors $\underline{x}$ and u satisfy

$$r := \|\underline{x}\| = \|u\|^2 = \mathbf{u}\;\bar{\mathbf{u}}\,. \tag{33}$$

Proof: By appropriately combining the two conjugations and using the rules (23), (24), (27), (28), (30) we obtain

$$\|\underline{x}\|^2 = \mathbf{x}\;\bar{\mathbf{x}} = \mathbf{u}\,(\mathbf{u}^\star\;\bar{\mathbf{u}}^\star)\;\bar{\mathbf{u}} = |\mathbf{u}^\star|^2\;|\,\mathbf{u}\,|^2 = |\,\mathbf{u}\,|^4 = \|u\|^4\;,$$

from where the statement follows. □

4.3 The Inverse Map

Since the mapping (32) does not preserve the dimension its inverse in the usual sence does not exist. However, the present quaternion formalism yields an elegant way of finding the corresponding *fibration* of the original space $\mathbb{R}^4$. Being given a quaternion $\mathbf{x} = x_0 + i\,x_1 + j\,x_2$ with vanishing k-component, $\mathbf{x} = \mathbf{x}^\star$, we want to find all quaternions $\mathbf{u}$ such that $\mathbf{u}\,\mathbf{u}^\star = \mathbf{x}$. We propose the following solution in two steps:

First step: Find a particular solution $\mathbf{u} = \mathbf{v} = \mathbf{v}^\star = v_0 + i\,v_1 + j\,v_2$ which has also a vanishing k-component. Since $\mathbf{v}\,\mathbf{v}^\star = \mathbf{v}^2$ we may use Equ. (21), which was developed for the complex square root, also for the square root of a quaternion:

$$\mathbf{v} = \frac{\mathbf{x} + |\mathbf{x}|}{\sqrt{2\,\left(|\mathbf{x}| + x_0\right)}}\ .$$

Clearly, $\mathbf{v}$ has a vanishing k-component.

Second step: The entire family of solutions (the fibre corresponding to $\mathbf{x}$, geometrically a circle in $\mathbb{R}^4$ parametrized by the angle ϑ), is given by

$$\mathbf{u} = \mathbf{v} \cdot e^{k\,\vartheta} = \mathbf{v}\,(\cos\vartheta + k\sin\vartheta)\,.$$

Proof. $\mathbf{u}\,\mathbf{u}^\star = \mathbf{v}\,e^{k\,\vartheta}\,e^{-k\,\vartheta}\,\mathbf{v}^\star = \mathbf{v}\,\mathbf{v}^\star = \mathbf{x}\,.$ □

4.4 The Regularization Procedure with Quaternions

In order to regularize the perturbed three-dimensional Kepler motion by means of the KS transformation it is necessary to look at the properties of the map (31) under differentiation.

The transformation (31) or (32) is a mapping from $\mathbb{R}^4$ to $\mathbb{R}^3$; it therefore leaves one degree of freedom in the parametric space undetermined. In KS theory (Kustaanheimo and Stiefel, 1965; Stiefel and Scheifele, 1971), this freedom is taken advantage of by trying to inherit as much as possible of the conformality properties of the Levi-Civita map, but other approaches exist (e.g., Vrbik 1995). By imposing the "bilinear relation"

$$2\,(u_3\,du_0 - u_2\,du_1 + u_1\,du_2 - u_0\,du_3) = 0 \tag{34}$$

between the vector $u = (u_0, u_1, u_2, u_3)$ and its differential du on orbits the tangential map of (32) becomes a linear map with an orthogonal (but non-normalized) matrix.

This property has a simple consequence on the differentiation of the quaternion representation (31) of the KS transformation. Considering the noncommutativity of the quaternion product, the differential of Equ. (31) becomes

$$d\mathbf{x} = d\mathbf{u} \cdot \mathbf{u}^\star + \mathbf{u} \cdot d\mathbf{u}^\star \,, \tag{35}$$

whereas (34) takes the form of a commutator relation,

$$\mathbf{u} \cdot d\mathbf{u}^\star - d\mathbf{u} \cdot \mathbf{u}^\star = 0 \,. \tag{36}$$

Combining (35) with the relation (36) yields the elegant result

$$d\mathbf{x} = 2\, \mathbf{u} \cdot d\mathbf{u}^\star \,, \tag{37}$$

i.e. the bilinear relation (34) of KS theory is equivalent with the requirement that the tangential map of $\mathbf{u} \mapsto \mathbf{u}\,\mathbf{u}^\star$ behaves as in a commutative algebra.

By using the tools collected in this section together with the differentiation rule (37) the regularization procedure outlined in Section 3 will now be carried out for the three-dimensional Kepler problem. Care must be taken to preserve the order of the factors in quaternion products. Exchanging two factors is permitted if one of the factors is real or if the factors are mutually conjugate. An important tool for simplifying expressions is regrouping factors of multiple products according to the associative law (24). In order to display the simplicity of this approach we present all the details of the formal computations.

(a) First step in space: Slow-motion movie

Let $\mathbf{x} = x_0 + i\, x_1 + j\, x_2 \in \mathbb{U}$ be the quaternion associated with the position vector $\underline{x} = (x_0, x_1, x_2) \in \mathbb{R}^3$; then the unperturbed Kepler problem (3) in space, written in quaternion notation, is given by

$$\ddot{\mathbf{x}} + \mu \frac{\mathbf{x}}{r^3} = 0 \in \mathbb{U} \,, \quad r = |\mathbf{x}| \,. \tag{38}$$

The first transformation step calls for introducing the fictitious time τ according to Equ. (11). We restrict ourselves to Sundman's choice $c = 1$, hence $dt = r \cdot d\tau$. The results are formally identical with Equ. (13) with $c = 1$,

$$r\, \mathbf{x}'' - r'\, \mathbf{x}' + \mu\, \mathbf{x} = 0 \,, \qquad \frac{1}{2\, r^2}\, |\mathbf{x}'|^2 - \frac{\mu}{r} = -h \,. \tag{39}$$

(b) Second step: KS transformation with quaternions

Instead of the conformal squaring according to Equ. (14) we use the KS transformation (31),

$$\mathbf{x} = \mathbf{u}\,\mathbf{u}^\star\,, \qquad r := |\mathbf{x}| = \mathbf{u}\,\bar{\mathbf{u}}\,. \tag{40}$$

Differentiation by means of the commutator relation (36) yields

$$\mathbf{x}' = 2\,\mathbf{u}\,\mathbf{u}^{\star\,\prime}\,, \quad \mathbf{x}'' = 2\,\mathbf{u}\,\mathbf{u}^{\star\,\prime\prime} + 2\,\mathbf{u}'\,\mathbf{u}^{\star\,\prime}\,, \quad r' = \mathbf{u}'\,\bar{\mathbf{u}} + \mathbf{u}\,\bar{\mathbf{u}}'\,. \tag{41}$$

Substitution of (40) and (41) into (39_1) results in the lengthy equation

$$(\mathbf{u}\,\bar{\mathbf{u}})\,(2\,\mathbf{u}\,\mathbf{u}^{\star\,\prime\prime} + 2\,\mathbf{u}'\,\mathbf{u}^{\star\,\prime}) - (\mathbf{u}'\,\bar{\mathbf{u}} + \mathbf{u}\,\bar{\mathbf{u}}')\,2\,\mathbf{u}\,\mathbf{u}^{\star\,\prime} + \mu\,\mathbf{u}\,\mathbf{u}^\star = 0\,, \tag{42}$$

which is considerably simplified by observing that the second and third term – after applying the distributive law – compensate:

$$2\,(\mathbf{u}\,\bar{\mathbf{u}})\,\mathbf{u}'\,\mathbf{u}^{\star\,\prime} \;-\; 2\,\mathbf{u}'\,(\bar{\mathbf{u}}\,\mathbf{u})\,\mathbf{u}^{\star\,\prime} \;=\; 0\,.$$

Furthermore, by means of (23), (24) and (36) the fourth term of (42) may be simplified as follows:

$$-2\,(\mathbf{u}\,\bar{\mathbf{u}}')\,(\mathbf{u}\,\mathbf{u}^{\star\,\prime}) \;=\; -\,2\,\mathbf{u}\,(\bar{\mathbf{u}}'\,\mathbf{u}')\,\mathbf{u}^\star \;=\; -\,2\,|\,\mathbf{u}'|^2\,\mathbf{u}\,\mathbf{u}^\star\,.$$

By using this and left-dividing by $\mathbf{u}$ Equ. (42) now becomes

$$2\,r\,\mathbf{u}^{\star\,\prime\prime} + (\,\mu - 2\,|\mathbf{u}'|^{\,2}\,)\,\mathbf{u}^\star = 0\,, \tag{43}$$

in almost perfect formal agreement with Equ. (17) (with $c = 1$) of the planar case.

(c) Third step: Fixing the energy in space

From (41), (30), (33) we have

$$|\,\mathbf{x}'\,|^2 = \mathbf{x}'\,\bar{\mathbf{x}}' = 4\,\mathbf{u}\,(\,\mathbf{u}^{\star\,\prime}\,\bar{\mathbf{u}}^{\star\,\prime}\,)\,\bar{\mathbf{u}} = 4\,r\,|\,\mathbf{u}'\,|^{\,2}\,; \tag{44}$$

therefore Equ. (39_2) becomes

$$\mu - 2\,|\,\mathbf{u}'\,|^2 \;=\; r\,h \tag{45}$$

in formal agreement with Equ. (18) found for the planar case. Substituting this into the star-conjugate of (43) and dividing by r yields the elegant final result

$$2\,\mathbf{u}'' \;+\; h\,\mathbf{u} = 0\,, \tag{46}$$

a differential equation in perfect agreement with the result found in the planar case.

5 The Perturbed Spatial Kepler Problem

We now consider the perturbed spatial Kepler problem,

$$\ddot{\mathbf{x}} + \mu \frac{\mathbf{x}}{r^3} = \varepsilon\, \mathbf{f}(\mathbf{x}, t)\,, \quad r = |\, \mathbf{x}\,|\,, \tag{47}$$

written in quaternion notation. $\mathbf{f}(\mathbf{x}, t)$ is the perturbing function, $\mathbf{x} \in \mathbb{U}$ and $\mathbf{f} \in \mathbb{U}$ are quaternions with vanishing k-components, and ε is a small parameter. Note that in the perturbed case an energy equation formally identical with (9) still holds. However, $h = h(t)$ and $a = a(t)$ are now slowly varying functions of time, $a(t)$ being the *osculating* major semi-axis; $h(t)$ satisfies the differential equation

$$\dot{h} = -\,\langle \dot{x},\, \varepsilon\, f \rangle \quad \text{or} \quad h' = -\,\langle x',\, \varepsilon\, f \rangle\,, \tag{48}$$

where $\langle \cdot\,, \cdot \rangle$ denotes the dot product of 3-vectors.

In the following, we report the results of the regularization procedure outlined in Section 4. The details are left to the reader as an exercise. Step 1 with $c = 1$ yields

$$r\, \mathbf{x}'' - r'\, \mathbf{x}' + \mu\, \mathbf{x} = r^3\, \varepsilon\, \mathbf{f}(\mathbf{x}, t)$$

instead of Equ. (39_1). By using (44) the energy equation (39_2) again becomes

$$\mu - 2\,|\, \mathbf{u}'\,|^2 = r\, h\,.$$

The right-hand side of Equ. (42) becomes

$$\mathbf{u}\, \bar{\mathbf{u}}\, r^2\, \varepsilon\, \mathbf{f}(\mathbf{x}, t)$$

instead of 0. Simplification as in Section 4 as well as left-multiplication by $r^{-1}\, \mathbf{u}^{-1}$ and star conjugation finally yields the perturbing equation for the quaternion coordinate $\mathbf{u}$:

Theorem 2: KS regularization, as formulated in terms of quaternions in Section 4, transforms the perturbed Kepler problem (47) into the perturbed harmonic oscillator

$$2\, \mathbf{u}'' + h\, \mathbf{u} = r\, \varepsilon\, \mathbf{f}(\mathbf{x}, t)\, \bar{\mathbf{u}}^\star\,, \quad r = |\, \mathbf{u}\,|^2\,,$$

where $h = r^{-1}\,(\mu - 2\,|\, \mathbf{u}'\,|^2)$ is the negative of the (slowly varying) energy. □

In the following summary we collect the complete set of differential equations defining the regularized system equivalent to the perturbed spatial Kepler problem (47). The harmonic oscillator of Theorem 2 appears in the first line. For stating an initial-value problem a starting value of $\mathbf{u}$ needs to be chosen according to Section 4.3. The corresponding initial velocity is obtained by solving (37) for $d\mathbf{u}$:

$$\frac{d\mathbf{u}}{d\tau} = \frac{1}{2\,r}\,\frac{d\mathbf{x}}{dt}\,\bar{\mathbf{u}}^\star\,.$$

Summary. Regularized system for the 3D perturbed Kepler problem (47).

$$\begin{aligned} 2\,\mathbf{u}'' + h\,\mathbf{u} &= r\,\varepsilon\,\mathbf{f}(\mathbf{x},t)\,\bar{\mathbf{u}}^\star\,, & r = |\,\mathbf{u}\,|^2,\quad (\,)' = \frac{d}{d\tau} \\ t' &= r\,, & \mathbf{x} = \mathbf{u}\,\mathbf{u}^\star \\ h' &= -\varepsilon\,\langle\, x', f(\mathbf{x},t)\,\rangle \quad \text{or} & h = r^{-1}\,(\mu - 2\,|\mathbf{u}'|^2) \end{aligned} \tag{49}$$

Remark. Introducing the *osculating* eccentric anomaly E by $dE = \sqrt{2\,h}\,d\tau$ transforms the first differential equation into

$$4\,\mathbf{u}'' + \mathbf{u} = \frac{\varepsilon}{h}\,\Big(r\,\mathbf{f}(\mathbf{x},t)\,\bar{\mathbf{u}}^\star + 2\,\langle\, x', f(\mathbf{x},t)\,\rangle\,\mathbf{u}'\Big)\,, \tag{50}$$

a perturbed harmonic oscillator with constant frequency $\omega = \frac{1}{2}$. As of here $(\,)' = d/dE$. This equation is particularly well suited for introducing orbital elements with simple pertubation equations.

5.1 Osculating Elements

Consider the scalar differential equation

$$4\,u'' + u = g\,,\quad u \in \mathbb{R} \tag{51}$$

as a model for the system (50) of differential equations, where g stands for a small perturbation, e.g., the right-hand side of (50). With $v := 2\,u'$ Equ. (51) may be written as

$$\begin{pmatrix} u \\ v \end{pmatrix}' = A \begin{pmatrix} u \\ v \end{pmatrix} + \begin{pmatrix} 0 \\ g/2 \end{pmatrix} \quad \text{with} \quad A = \begin{pmatrix} 0 & 1/2 \\ -1/2 & 0 \end{pmatrix}\,. \tag{52}$$

A matrix solution $U(E)$ of the unperturbed problem $U' = A\,U$ is

$$U(E) = \exp(A\,E) = \begin{pmatrix} \cos(\frac{E}{2}) & \sin(\frac{E}{2}) \\ -\sin(\frac{E}{2}) & \cos(\frac{E}{2}) \end{pmatrix} .$$

We finally solve the perturbed system (50) by the method of *variation of the constant*. We seek a solution of the form

$$\begin{pmatrix} u(E) \\ v(E) \end{pmatrix} = U(E) \begin{pmatrix} a(E) \\ b(E) \end{pmatrix} ,$$

where $a(E), b(E)$ are the slowly varying orbital elements. Substituting this and its derivative into the vector differential equation (52) and solving for the derivatives of the elements yields the differential equations for the *osculating orbital elements* as functions of the eccentric anomaly E:

$$\begin{aligned} \frac{d\mathbf{a}}{dE} &= -\frac{\mathbf{g}}{2} \cdot \sin(\frac{E}{2}) \\ \frac{d\mathbf{b}}{dE} &= \frac{\mathbf{g}}{2} \cdot \cos(\frac{E}{2}) . \end{aligned} \tag{53}$$

Here we have used bold face symbols in order to indicate that the above differential equations for the osculating orbital elements not only hold for scalars $a, b, u, g \in \mathbb{R}$, but also for quaternions $\mathbf{a}, \mathbf{b}, \mathbf{u}, \mathbf{g} \in \mathbb{U}$, as well as for vectors $\vec{a}, \vec{b}, \vec{u}, \vec{g} \in \mathbb{R}^n,\ n \in \mathbb{N}$.

The final pertubation equations may be obtained by using $dE = \sqrt{2\,h}\,d\tau$ and (50) in order to transform the system (49) to differentiations with respect to E instead of τ. Furthermore, the equation (50) in the first line must be replaced by the system (53). In this form the equatins of motion are well suited for numerical purposes. Series expansions may easily be obtained for perturbations not depending explicitly on time.

Conclusions

- The classical regularizations by Levi-Civita or Kustaanheimo-Stiefel transform the equations of motion of the planar or spatial Kepler problem into the linear differential equations of a harmonic oscillator in 2 or 4 dimensions, respectively.

- Based on this, we are able to formulate a simple and concise perturbation theory of the Kepler problem.
- The "language" of quaternions allows for a concise formalism for developing the Kustaanheimo-Stiefel theory of regularization of the spatial Kepler problem.
- The use of the *"star-conjugate"* $\mathbf{u}^\star$ of a quaternion $\mathbf{u}$ according to

  $$\mathbf{u} = u_0 + i\,u_1 + j\,u_2 + k\,u_3\,, \quad \mathbf{u}^\star = u_0 + i\,u_1 + j\,u_2 - k\,u_3$$

  yields a spatial regularization theory in perfect formal agreement with Levi-Civita's planar regularization using complex variables.

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