Quaternions and the Perturbed Kepler Problem

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Abstract. Quaternions, introduced by W. R. Hamilton (1844) as a generalization of complex numbers, lead to a remarkably simple representation of the perturbed three-dimensional Kepler problem as a perturbed harmonic oscillator. The paper gives an overview of this technique, including an outlook to applications in perturbation theories.

Key words: Perturbed Kepler problem, Kustaanheimo-Stiefel regularization, quaternions, Birkhoff transformation.

1. Introduction

A large branch of celestial mechanics is concerned with handling perturbations of the Kepler problem, described by a strongly nonlinear differential equation for the vector $x \in \mathbb{R}^n$, n = 2, 3 as a function of time t,

$$\ddot{x} + \mu \frac{x}{r^3} = \varepsilon f(x, t), \quad r = \|x\|, \tag{1}$$

where x is the position vector of the moving particle with respect to the central body (with gravitational parameter $\mu > 0$), dots denote derivatives with respect to t, and $\varepsilon f(x, t)$ is a given small perturbation.

As will be demonstrated in the example below, the linearity of a problem leads to formally simple perturbation theories. Fortunately, there exist sets of variables in which the Kepler problem becomes linear; these are preferred variables for treating perturbed Kepler problems.

In this paper we will revisit two closely related sets of variables that were introduced in order to regularize the collision singularity in the Kepler problem: the variables introduced by Levi-Civita (1920), in which the planar Kepler problem appears as a harmonic oscillator in two dimensions, and the KS variables (Kustaanheimo 1964, Kustaanheimo and Stiefel 1965), in which the spatial Kepler problem appears as a harmonic oscillator in four dimensions. Both sets of variables have therefore the agreeable property of transforming the differential equations of the Kepler problem into a system of linear differential equations; they are therefore good variables for formulating theories of the perturbed Kepler problem. We will present a unified treatment of

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these two classical topics, using complex variables in the planar case and quaternions in the three-dimensional case. For completeness we mention that in a set of variables based on radial inversion in momentum space (see, e.g., Siegel and Moser, 1971, or the summary in Celletti, 2002) the Kepler problem also becomes linear.

The use of quaternions for the purpose of regularization of the Kepler problem in three dimensions has been contemplated before. In the comprehensive text by Stiefel and Scheifele (1971) the use of quaternions was taken into consideration (p. 286), but clearly rejected: "Any attempt to substitute the theory of the KS matrix by the more popular theory of the quaternion matrices leads to failure or at least to a very unwieldy formalism." Almost simultaneously, Maria Dina Vivarelli (1994) and Jan Vrbik (1994, 1995) demonstrated the usefulness of quaternions in this field. Here we will describe a new, elegant way of handling the three-dimensional case in complete analogy to the well-known planar case by introducing an unconventional conjugation of quaternions (see the definition in Equ. (24) below), first mentioned by Waldvogel (2006).

Perturbation theories of ordinary differential equations are comparatively simple for linear problems. Consider, e.g., the perturbed system

$$\dot{x}(t) + A(t)x(t) - b(t) = \varepsilon f(x,t), \quad x : t \in \mathbb{R} \mapsto x(t) \in \mathbb{R}^n, \quad (2)$$

of linear differential equations, where A(t) is a given time-dependent matrix. Equ. (2) 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

$$\dot{x}_k(t) + A(t) x_k(t) = f_{k-1}(t), \quad k = 0, 1, 2, \dots$$
 (3)

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

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

Note that the linear differential equations (3) are all of the type of the unperturbed problem k = 0; they only differ in their right-hand sides.

In Section 2 Levi-Civita's regularization procedure in complex notation will be summarized. Section 3 contains a brief introduction to quaternion algebra and states the KS transformation in quaternion notation. In Section 4, the main part of this paper, we develop a simple, concise way of transforming the spatial perturbed Kepler problem into a perturbed harmonic oscillator in 4 dimensions. As a byproduct, an elegant representation of the spatial Birkhoff transformation in quaternion notation will be given in Section 5.

2. The Levi-Civita Transformation

Here we summarize the *three* steps necessary for regularizing (and thus "linearizing") the perturbed planar Kepler problem by Levi-Civita's transformation. Throughout this section we use complex notation, i.e. instead of the vectors $x = (x_1, x_2)^T \in \mathbb{R}^2$, $f = (f_1, f_2)^T$ we use the corresponding complex numbers $\mathbf{x} = x_1 + i x_2 \in \mathbb{C}$, $\mathbf{f} = f_1 + i f_2 \in \mathbb{C}$.

2.1. FIRST STEP: SLOW-MOTION MOVIE

Instead of the physical time t a new independent variable τ , called the fictitious time, is introduced by the differential relation

$$dt = r \cdot d\tau, \quad \frac{d}{d\tau}(\) = (\)'. \tag{4}$$

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

$$\frac{d}{dt} = \frac{1}{r} \frac{d}{d\tau}, \quad \frac{d^2}{dt^2} = \frac{1}{r^2} \frac{d^2}{d\tau^2} - \frac{r'}{r^3} \frac{d}{d\tau}$$

Equ. (1) transforms into

$$r \mathbf{x}'' - r' \mathbf{x}' + \mu \mathbf{x} = r^3 \varepsilon \mathbf{f} \in \mathbb{C} .$$
 (5)

2.2. 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 $\mathbf{u} = u_1 + i \, u_2 \in \mathbb{C}$,

$$\mathbf{x} = \mathbf{u}^2 , \qquad (6)$$

i.e. the mapping from the parametric plane to the physical plane is chosen as a conformal squaring. This is based on the observation that conformal squaring maps an origin-centered ellipse to a Keplerian ellipse with one focus at the origin (see Fig 1). Equ. (6) implies

$$r = |\mathbf{x}| = |\mathbf{u}|^2 = \mathbf{u}\bar{\mathbf{u}}, \qquad (7)$$



Figure 1. The image of a (doubly covered) Keplerian ellipse with one focus at the origin of the physical plane (left) under the conformal square root is an ellipse centered at the origin of the parametric plane (right)

and differentiation of Equs. (6) and (7) yields

$$\mathbf{x}' = 2 \mathbf{u} \mathbf{u}' , \quad \mathbf{x}'' = 2 \left(\mathbf{u} \mathbf{u}'' + \mathbf{u}'^2 \right) \in \mathbb{C} , \quad r' = \mathbf{u}' \,\overline{\mathbf{u}} + \mathbf{u} \,\overline{\mathbf{u}}' . \quad (8)$$

By substituting this into (5), cancelling two equal terms $(2r \mathbf{u}'^2 \text{ and } 2\mathbf{u}' \mathbf{\bar{u}} \mathbf{u} \mathbf{u}')$ and dividing by \mathbf{u} we obtain

$$2r\mathbf{u}'' + (\mu - 2|\mathbf{u}'|^2)\mathbf{u} = r^2\bar{\mathbf{u}}\varepsilon\mathbf{f}.$$
(9)

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

$$\sqrt{\mathbf{x}} = \frac{\mathbf{x} + |\mathbf{x}|}{\sqrt{2\left(|\mathbf{x}| + \operatorname{Re}\mathbf{x}\right)}} \tag{10}$$

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 (10) in the upper half-plane; it therefore provides the analytic continuation of (10) into the sector $\pi \leq \arg(\mathbf{x}) < 2\pi$. Furthermore, it avoids a loss of accuracy near the negative real axis $\mathbf{x} < 0$.

2.3. Third step: Fixing the energy

This step is simple for the unperturbed problem, $\varepsilon = 0$. Integrating the inner product of Equ. (1) and the vector $\dot{x} \in \mathbb{R}^2$ yields the well-known energy equation

$$\frac{1}{2} \| \dot{x} \|^2 - \frac{\mu}{r} = -h = \text{const.}$$
(11)

where the energy constant h is chosen such that h > 0 corresponds to an elliptic orbit. From (4) and (8) there follows (using again complex notation):

$$\dot{\mathbf{x}} = \frac{1}{r} \cdot 2 \,\mathbf{u} \,\mathbf{u}', \quad \frac{1}{2} \,|\, \dot{\mathbf{x}}\,|^2 = 2 \,\frac{|\,\mathbf{u}'\,|^2}{r}\,, \tag{12}$$

and (11) implies

$$\mu - 2 |\mathbf{u}'|^2 = r h.$$
(13)

Substituting this into (9) and dividing by r yields

$$2\mathbf{u}'' + h\mathbf{u} = 0, \qquad (14)$$

a system of linear differential equations describing a harmonic oscillator in two dimensions with frequency $\omega = \sqrt{h/2}$.

In the perturbed case h of Equ. (11) is no longer a constant, but is a slowly varying function and satisfies the differential equation

$$\dot{h} = -\langle \dot{x}, \varepsilon f \rangle$$
 or $h' = -\langle x', \varepsilon f \rangle$, (15)

where $\langle x, y \rangle$ denotes the inner product of the vectors $x, y \in \mathbb{R}^2$. The energy equation (13) still holds, and instead of (14) we obtain

$$2\mathbf{u}'' + h\mathbf{u} = |\mathbf{u}|^2 \,\bar{\mathbf{u}} \,\varepsilon \,\mathbf{f} \,. \tag{16}$$

Remark. Equation (16), together with the second equation (15), describes a perturbed harmonic oscillator with slowly varying frequency; it may be transformed to constant frequency by introducing a new independent variable s proportional to the osculating eccentric anomaly, e.g., according to the differential relation

$$ds = \sqrt{h} \, d\tau$$
 .

This results in the system of differential equations

$$rac{dh}{ds} = -rac{r}{\sqrt{h}} \left\langle \dot{x}, arepsilon f
ight
angle, \qquad 2 \; rac{d^2 \mathbf{u}}{ds^2} \; + \; \mathbf{u} = rac{r}{h} \, ar{\mathbf{u}} \; arepsilon \mathbf{f} \; - \; rac{1}{h} rac{dh}{ds} rac{d \mathbf{u}}{ds} \; .$$

For more details regarding applications to perturbation theories see Waldvogel (2006).

3. Quaternion Algebra and the KS Transformation

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 2.2 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 discovered already 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 twobody problem. Quaternion algebra, introduced by W. R. Hamilton (1844), turns out to be very well suited as a tool for regularizing the three-dimensional Kepler motion, as was observed by M. D. Vivarelli (1994) and J. Vrbik (1994, 1995). Here we will present a new elegant way of extending the Levi-Civita regularization to three dimensions by means of quaternions.

3.1. 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

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

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

$$\mathbf{u} = u_0 + i\,u_1 + j\,u_2 + k\,u_3 \tag{17}$$

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:

$$c \mathbf{u} = \mathbf{u} c, \quad c \in \mathbb{R}, \quad \mathbf{u} \in \mathbb{U},$$
(18)

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

$$\left(\mathbf{u}\,\mathbf{v}\right)\mathbf{w} = \mathbf{u}\left(\mathbf{v}\,\mathbf{w}\right).\tag{19}$$

The quaternion **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 $\vec{i} = (i, j, k)$; the quaternion **u** may then be written formally as $\mathbf{u} = u_0 + \langle \vec{i}, \vec{u} \rangle$. For the two quaternion products of **u** and $\mathbf{v} = v_0 + \langle \vec{i}, \vec{v} \rangle$ we then obtain the concise expressions

$$\mathbf{u} \mathbf{v} = u_0 v_0 - \langle \vec{u}, \vec{v} \rangle + \langle \vec{i}, u_0 \vec{v} + v_0 \vec{u} + \vec{u} \times \vec{v} \rangle$$

$$\mathbf{v} \mathbf{u} = u_0 v_0 - \langle \vec{u}, \vec{v} \rangle + \langle \vec{i}, u_0 \vec{v} + v_0 \vec{u} - \vec{u} \times \vec{v} \rangle,$$
(20)

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

$$\bar{\mathbf{u}} = u_0 - i \, u_1 - j \, u_2 - k \, u_3 \,; \tag{21}$$

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

$$|\mathbf{u}|^2 = \mathbf{u}\,\bar{\mathbf{u}} = \bar{\mathbf{u}}\,\mathbf{u} = \sum_{l=0}^3 u_l^2\,.$$
(22)

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

$$\overline{\mathbf{u}\,\mathbf{v}} = \bar{\mathbf{v}}\,\bar{\mathbf{u}}\,.\tag{23}$$

3.2. The KS Transformation with quaternions

Here we will revisit KS regularization and present a new, elegant derivation of it, using quaternion algebra and an unconventional "conjugate" \mathbf{u}^* referred to as the *star conjugate* of the quaternion $\mathbf{u} = u_0 + i u_1 + j u_2 + k u_3$:

$$\mathbf{u}^{\star} := u_0 + i \, u_1 + j \, u_2 - k \, u_3 \,. \tag{24}$$

The star conjugate of ${\bf u}$ may be expressed in terms of the conventional conjugate $\bar{{\bf u}}$ as

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

however, it turns out that the definition (24) leads to a particularly elegant treatment of KS regularization. The following elementary properties are easily verified:

$$\begin{aligned} (\mathbf{u}^{\star})^{\star} &= \mathbf{u} \\ |\mathbf{u}^{\star}|^2 &= |\mathbf{u}|^2 \\ (\mathbf{u}\,\mathbf{v})^{\star} &= \mathbf{v}^{\star}\,\mathbf{u}^{\star} \,. \end{aligned}$$
 (25)

Consider now the mapping

$$\mathbf{u} \in \mathbb{U} \longmapsto \mathbf{x} = \mathbf{u} \, \mathbf{u}^{\star} \,. \tag{26}$$

Star conjugation immediately yields $\mathbf{x}^* = (\mathbf{u}^*)^* \mathbf{u}^* = \mathbf{x}$; 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

$$\begin{aligned}
x_0 &= u_0^2 - u_1^2 - u_2^2 + u_3^2 \\
x_1 &= 2(u_0 u_1 - u_2 u_3) \\
x_2 &= 2(u_0 u_2 + u_1 u_3),
\end{aligned}$$
(27)

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

$$r := \|\underline{x}\| = \|u\|^2 = \mathbf{u} \, \bar{\mathbf{u}} \,.$$
 (28)

Proof: By appropriately combining the two conjugations and using the rules (18), (19), (22), (23), (25) we obtain

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

from where the statement follows.

3.3. The inverse map

Since the mapping (27) 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, $\mathbf{x} = \mathbf{x}^*$, we want to find all quaternions \mathbf{u} such that $\mathbf{u} \mathbf{u}^* = \mathbf{x}$. We propose the following solution in two steps:

First step: Find a particular solution $\mathbf{u} = \mathbf{v} = \mathbf{v}^* = v_0 + i v_1 + j v_2$ which has also a vanishing k-component. Since $\mathbf{v} \mathbf{v}^* = \mathbf{v}^2$ we may use Equ. (10), which was developed for the complex square root, also for the square root of a quaternion:

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

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 φ), is given by

$$\mathbf{u} = \mathbf{v} \cdot e^{k\varphi} = \mathbf{v} \left(\cos \varphi + k \sin \varphi \right).$$

Proof. $\mathbf{u} \mathbf{u}^* = \mathbf{v} e^{k\varphi} e^{-k\varphi} \mathbf{v}^* = \mathbf{v} \mathbf{v}^* = \mathbf{x}.$

4. KS Regularization 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 (26) under differentiation.

The transformation (26) or (27) 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"

$$2(u_3 du_0 - u_2 du_1 + u_1 du_2 - u_0 du_3) = 0$$
⁽²⁹⁾

between the vector $u = (u_0, u_1, u_2, u_3)$ and its differential du on orbits the tangential map of (27) becomes a linear map with an orthogonal (but non-normalized) matrix. This property has a simple consequence on the differentiation of the quaternion representation (26) of the KS transformation. Considering the noncommutativity of the quaternion product, the differential of Equ. (26) becomes

$$d\mathbf{x} = d\mathbf{u} \cdot \mathbf{u}^{\star} + \mathbf{u} \cdot d\mathbf{u}^{\star}, \qquad (30)$$

whereas (29) takes the form of a commutator relation,

$$\mathbf{u} \cdot d\,\mathbf{u}^{\star} - d\,\mathbf{u} \cdot \mathbf{u}^{\star} = 0\,. \tag{31}$$

Combining (30) with the relation (31) yields the elegant result

$$d\mathbf{x} = 2 \,\mathbf{u} \cdot d \,\mathbf{u}^{\star} \,, \tag{32}$$

i.e. the bilinear relation (29) of KS theory is equivalent with the requirement that the tangential map of $\mathbf{u} \mapsto \mathbf{u} \, \mathbf{u}^*$ behaves as in a commutative algebra.

By using the tools collected in Section 3 together with Equ. (32) the regularization procedure outlined in Section 2 will now be carried out for the three-dimensional perturbed 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 (19). In order to stress the simplicity of this approach we present all the details of the formal computations.

4.1. 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 perturbed Kepler problem (1) is given by

$$\ddot{\mathbf{x}} + \mu \, \frac{\mathbf{x}}{r^3} = \varepsilon \, \mathbf{f}(\mathbf{x}, t) \in \mathbb{U} \,, \quad r = |\mathbf{x}| \,, \tag{33}$$

where $\mathbf{f}(\mathbf{x},t) = f_0(\mathbf{x},t) + i f_1(\mathbf{x},t) + j f_2(\mathbf{x},t) = \mathbf{f}^*(\mathbf{x},t)$ is the quaternion associated with the perturbation $\underline{f}(\underline{x},t) \in \mathbb{R}^3$.

The first transformation step calls for introducing the fictitious time τ according to Equ. (4), $dt = r \cdot d\tau$; the result is formally identical with Equ. (5),

$$r \mathbf{x}'' - r' \mathbf{x}' + \mu \mathbf{x} = r^3 \varepsilon \mathbf{f} \in \mathbb{U}$$
. (34)

4.2. Second step: KS transformation with quaternions

Instead of the conformal squaring according to Equ. (6) we use the KS transformation (26),

$$\mathbf{x} = \mathbf{u} \, \mathbf{u}^{\star} \,, \qquad r := |\mathbf{x}| = \mathbf{u} \, \bar{\mathbf{u}} \,. \tag{35}$$

Differentiation by means of the commutator relation (31) yields

$$\mathbf{x}' = 2 \mathbf{u} \mathbf{u}^{\star'}, \quad \mathbf{x}'' = 2 \mathbf{u} \mathbf{u}^{\star''} + 2 \mathbf{u}' \mathbf{u}^{\star'}, \quad r' = \mathbf{u}' \bar{\mathbf{u}} + \mathbf{u} \bar{\mathbf{u}}'. \quad (36)$$

Substitution of (35) and (36) into (34) results in the lengthy equation

$$(\mathbf{u}\,\bar{\mathbf{u}})\left(2\,\mathbf{u}\,\mathbf{u^{\star}}''+2\,\mathbf{u}'\,\mathbf{u^{\star}}'\right)-\left(\mathbf{u}'\,\bar{\mathbf{u}}+\mathbf{u}\,\bar{\mathbf{u}}'\right)2\,\mathbf{u}\,\mathbf{u^{\star}}'+\mu\,\mathbf{u}\,\mathbf{u^{\star}}=r^{3}\,\varepsilon\,\mathbf{f}\,,\ (37)$$

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

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

Furthermore, by means of (18), (19) and (31) the fourth term of (37) may be simplified as follows:

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

By using this and left-dividing by \mathbf{u} Equ. (37) now becomes

$$2r \mathbf{u}^{\star''} + (\mu - 2|\mathbf{u}'|^2) \mathbf{u}^{\star} = r^2 \bar{\mathbf{u}} \varepsilon \mathbf{f}$$
(38)

in almost perfect formal agreement with Equ. (9) of the planar case.

4.3. Third step: Fixing the energy in space

In formal agreement with the planar case the energy equation expressed by fictitious time is

$$\frac{1}{2r^2} |\mathbf{x}'|^2 - \frac{\mu}{r} = -h \qquad \text{with} \qquad h' = -\langle \underline{x}', \varepsilon \underline{f} \rangle. \tag{39}$$

From (36), (25), (28) we have

$$|\mathbf{x}'|^2 = \mathbf{x}' \, \bar{\mathbf{x}}' = 4 \, \mathbf{u} \left(\mathbf{u}^{\star'} \, \bar{\mathbf{u}}^{\star'} \right) \bar{\mathbf{u}} = 4 \, r \, |\mathbf{u}'|^2 \,,$$

and the first equation of (39) becomes

$$\mu - 2 |\mathbf{u}'|^2 = rh \tag{40}$$

in formal agreement with Equ. (13) found for the planar case. Substituting this into the star-conjugate of (38) and dividing by r yields the elegant final result

$$2 \mathbf{u}'' + h \mathbf{u} = |\mathbf{u}|^2 \varepsilon \mathbf{f} \, \bar{\mathbf{u}}^{\star}, \qquad (41)$$

a differential equation in perfect agreement with (16) for the planar case; however, it takes more than an educated guess to get the correct right-hand side.

5. The Birkhoff Transformation

The topic of this section is not directly related to the preceding text; we add it here because the quaternion tools discussed before allow for an elegant representation of the spatial Birkhoff transformation.

This regularizing transformation was proposed by George David Birkhoff (1915), in order to regularize all singularities of the planar restricted three-body problem with a single transformation. Half a century later Stiefel and Waldvogel (1965) published a generalization of Birkhoff's transformation to three dimensions, using the KS transformation. Later these ideas were used by Waldvogel (1967a, 1967b).

Here we will first revisit the classical Birkhoff transformation (the same conformal map is known in aerodynamics as the Joukowsky transformation) and represent it as the composition of three elementary conformal mappings; this will then readily generalize to the spatial situation by means of quaternions.



Figure 2: The sequence of conformal maps generating the planar Birkhoff transformation

Consider a rotating physical plane parametrized by the complex variable $\mathbf{y} \in \mathbb{C}$; for convenience we assume the fixed primaries of the restricted three-body problem to be situated at the points A, C given by the complex posititons $\mathbf{y} = -1$ and $\mathbf{y} = 1$, respectively (see Figure 2). The complex variable of the parametric plane will be denoted by \mathbf{v} and will be normalized in such a way that the primaries are mapped to $\mathbf{v} = -1$ or $\mathbf{v} = 1$, respectively.

The key observation is that Levi-Civita's conformal map (6), $\mathbf{u} \mapsto \mathbf{x} = \mathbf{u}^2$, not only regularizes collisions at $\mathbf{x} = 0$ but also analogous singularities at $\mathbf{x} = \infty$. This is seen by closing the complex planes to become Riemann spheres (by adding the point at infinity) and using inversions $\mathbf{x} = 1/\tilde{\mathbf{x}}$, $\mathbf{u} = 1/\tilde{\mathbf{u}}$.

Taking advantage of this fact, we first map the \mathbf{v} -sphere to an auxiliary \mathbf{u} -sphere by the Möbius transformation

$$\mathbf{v} \longmapsto \mathbf{u} = \frac{\mathbf{v}+1}{\mathbf{v}-1} = 1 + \frac{2}{\mathbf{v}-1},$$
(42)

which takes the primaries A, C to the points $\mathbf{u} = 0$, $\mathbf{u} = \infty$, respectively. The Levi-Civita map (6) will leave these points invariant while regularizing collisions at A or C. Finally, the Möbius transformation

$$\mathbf{x} \mapsto \mathbf{y} = \frac{\mathbf{x}+1}{\mathbf{x}-1} = 1 + \frac{2}{\mathbf{x}-1}$$
 (43)

maps A, C to $\mathbf{y} = -1$ and $\mathbf{y} = 1$, respectively. The composition of the maps (42), (6), (43) yields

$$\mathbf{y} = \frac{\left(\frac{\mathbf{v}+1}{\mathbf{v}-1}\right)^2 + 1}{\left(\frac{\mathbf{v}+1}{\mathbf{v}-1}\right)^2 - 1} \quad \text{or} \quad \mathbf{y} = \frac{1}{2} \left(\mathbf{v} + \frac{1}{\mathbf{v}}\right), \quad (44)$$

the well known map used by Joukowsky and by Birkhoff.

In the spatial case we choose $\mathbf{v}, \mathbf{u}, \mathbf{x}, \mathbf{y} \in \mathbb{U}$ to be quaternions, $\mathbf{x} = \mathbf{x}^*, \ \mathbf{y} = \mathbf{y}^*$ being quaternions with vanishing k-components associated with 3-vectors $\underline{x}, \underline{y}$. Then the mappings (42), (43), now being shifted inversions in 4 or 3 dimensions, are both conformal maps, in fact the only conformal maps existing in those dimensions, except for the translations, magnifications, and rotations. Composing these with the KS or Hopf map (35), $\mathbf{u} \mapsto \mathbf{x} = \mathbf{u} \mathbf{u}^*$, yields

$$\mathbf{y} = 1 + (\mathbf{v}^{\star} - 1) (\mathbf{v} + \mathbf{v}^{\star})^{-1} (\mathbf{v} - 1)$$
 (45)

after a few lines of careful noncommutative algebra. This is easily split up into components by means of the inversion formula $1/\mathbf{v} = \bar{\mathbf{v}}/|\mathbf{v}|^2$; it agrees with the results of Stiefel and Waldvogel (1965) up to the sign of v_3 . Both transformations regularize; the discrepancy is due to the different definition of the orientation in the inversions.

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