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ABSTRACT

It is well-known that the equations of Keplerian motion suffer from being singular at collision. This is a definite disadvantage when one wants to integrate the perturbed Kepler problem for orbits which are close to collision, e. g. those of spacecraft moving from the Earth to the Moon or some other planet.

In order to overcome this difficulty, Kustaanheimo [1964] proposed a regularisation method, which was later applied by Kustaanheimo and Stiefel [1965] and others and is known in celestial mechanics under the (ugly) name "KS-(=Kustaanheimo-Stiefel-)transformation".

In this note, we shall show that there is an extremely elegant description of this procedure using quaternions, contrary to earlier belief (see, e. g., the monograph by Stiefel and Scheifele [1971], where the possibility of such an approach is denied).

This erroneous conclusion which is quite widespread in the literature stems from an unlucky choice of some sign in the above-mentioned book by Stiefel and Scheifele.

We think it will be worthwhile to demonstrate the power of the quaternionic variant of the method in question.

0. INTRODUCTION

Levi-Cività [1956] regularised the two-dimensional Kepler problem with the help of complex coordinates. He showed that a specific transformation of the time and a quadratic Ansatz in the complex coordinate suffices to reduce the equation of planar Kepler motion to a form which is free of singularities.

An exact three-dimensional counterpart of this transform, however, does not exist for topological reasons. Rather, one has to extend the parameter space to four dimensions, and introduce an additional restriction. The latter turns out to be quite natural.

This idea, due to Kustaanheimo and Stiefel, clearly suggests that it may be useful to describe the appropriate formulas in quaternions. It is therefore surprising that several authors, among them Stiefel himself, state that this is impossible. The main goal of the present paper is to correct this wrong statement.

We shall succeed in giving completely regular quaternionic equations which are equivalent to those discussed in Stiefel and Scheifele [1971], but are much simpler and more transparent.

Furthermore, we show that there is an intimate connection to the famous Hopf fibration. In conclusion, all of our results are very natural from a mathematical point of view.

1. ONE-DIMENSIONAL MOTION

In this paper, we shall discuss the motion of a particle, (henceforth called the "planet") in the gravitational field of some other body (the "sun"). All additional perturbative forces acting on the planet are assumed to be conservative; thus they can be derived from a suitable potential. The equation of motion thus reads in a coordinate system centered at the sun:

$$\vec{r} = -\frac{\mu}{r^3} r + \text{grad } V(r)$$
 (1)

where - as usual - derivatives with respect to the time t are denoted by dots, while μ is the product of Newton's gravitational constant with the solar mass. The perturbations are contained in the gradient of the potential V and will be supposed to depend in a known way on the planet's position vector r.

In the special case of one-dimensional motion (without restriction along the positive part of the x-axis of a Cartesian coordinate system), we can bring this relation to the form

$$\ddot{x} + \frac{\mu}{x^2} = \frac{dV}{dx}$$
(2)

The last formula can be integrated once, providing us with the energy equation

$$\frac{x^2}{2} = \frac{\mu}{x} + V(x) + E$$
(3)

where E is an integration constant, namely the energy per unit mass. This reduction is possible since we restricted ourselves to conservative perturbations. Most of the forces relevant to celestial mechanics possess this property.

Moreover, the regularisation procedure depends heavily on this fact; a more general treatment would be much more complicated and less elegant.

If a collision $(x \rightarrow 0)$ occurs, the potential gradient grad V is assumed to

remain finite. Under these circumstances, it is possible to regularise the equations by replacing the spatial coordinate x by some power u,

$$x = u^{\alpha}$$
 (4)

and the time t by a uniformising variable τ via the differential relation

$$dt = x^{\beta} d\tau$$
 (5)

Derivatives with respect to τ (called the **parametric time**) will be abbreviated by primes. Here α and β are constants which we have to determine such that the singularity for x = 0 disappears.

We first calculate the perturbation in the new coordinates, getting

$$\frac{dV}{dx} = \alpha^{-1} u^{1-\alpha} \frac{dV}{du}$$
(6)

Equally easily the velocity of the planet,

$$\dot{x} = u^{-\beta} x' = u^{-\beta} (\alpha u^{\alpha-1} u') = \alpha u^{\alpha-\beta-1} u'$$
 (7)

and its acceleration,

$$\ddot{x} = u^{-\beta} (u^{-\beta} x')' = \alpha u^{\alpha - 2\beta - 2} \left\{ u u'' + (\alpha - \beta - 1) (u')^2 \right\}$$
(8)

follow. The energy equation becomes after substitution .

$$\frac{1}{-\alpha^{2}}u^{2\alpha-2\beta-2}(u')^{2} = \mu u^{-\alpha} + V + E$$
(9)
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We solve for the square of u' and insert the result into the equation of motion. This leads to

$$\alpha u^{\alpha - 2\beta - 1} u'' + \left\{ 2 \alpha^{-1} (\alpha - \beta - 1) + 1 \right\} \mu u^{-2\alpha} + 2 \alpha^{-1} (\alpha - \beta - 1) \left[V(u) + E \right] u^{-\alpha} = \alpha^{-1} u^{1 - \alpha} \frac{dV}{du}$$
(10)

The collision corresponds to x = 0; in order to regularise we have to take α positive, otherwise we would shift the collision to infinity in u-space. But if $\alpha > 0$, the μ -term in (10) is the most singular, so it must be eliminated. This forces us to restrict the exponents α and β by the condition

$$2 \alpha^{-1} (\alpha - \beta - 1) + 1 = 0$$
 (11)

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$$\beta = \frac{3}{2}\alpha - 1 \tag{12}$$

The dynamical equation then simplifies considerably. We find

$$\alpha u^{-2\alpha+1} u'' - (V + E) u^{-\alpha} = \alpha^{-1} u^{1-\alpha} \frac{dV}{du}$$
(13)

which may also be written as

$$\alpha^2 u'' \simeq \alpha (V + E) u^{\alpha - 1} + u^{\alpha} \frac{dV}{du}$$
 (14)

In the absence of perturbations (V = 0), this is

$$\alpha u'' = E u^{\alpha - 1} \tag{15}$$

so clearly we have to set $\alpha = 2$, and consequently also $\beta = 2$, to make the last differential equation linear in u.

The general equation of perturbed one-dimensional motion then attains its final form,

 $2 u'' = (V + E) u + \frac{1}{2} u^2 \frac{dV}{du}$ (16)

while the energy conservation law reads

$$2 (u')^{2} = \mu + (V + E) u^{2}$$
(17)

2. THE HOPF FIBRATION

In order to calculate the third homotopy group $\pi_3(S^2)$ of the two-sphere S^2 , Hopf [1931,1935] attached a certain integer $\iota(f)$ to each C^{∞} -map

$$f: S^3 \longrightarrow S^2$$
 (18)

which is a homotopy invariant, i. e., is the same for homotopic maps. He found that this Hopf invariant $\iota(f)$ attains all integer values. In particular, he constructed a quadratic map

$$h: S^3 \longrightarrow S^2$$
(19)

as follows:

Let $P = (\alpha, \beta, \gamma, \delta)$ be a typical point on the (unit) 3-sphere

$$S^{3} = \left\{ (\alpha, \beta, \gamma, \delta) \in \mathbb{R}^{4} \mid \alpha^{2} + \beta^{2} + \gamma^{2} + \delta^{2} = 1 \right\}$$
(20)

which can also be written in complex coordinates

$$w_{1} = \alpha + \beta i \qquad (21)$$

and

$$w_{0} = \gamma + \delta i \qquad (22)$$

as

$$S^{3} = \left\{ \left(w_{1}, w_{2} \right) \in \mathbb{C}^{2} \quad \left| \quad \left| w_{1} \right|^{2} + \left| w_{2} \right|^{2} = 1 \right\}$$
(23)

The pair $(w_1, w_2) \neq (0, 0)$ can be considered as homogeneous coordinates of a point h(P) in projective space

$$\mathbb{P}^{1}(\mathbb{C}) = \mathbb{C} \cup \{\infty\} \cong \mathbb{S}^{2}$$
 (24)

via a stereographic projection. The Hopf map simply transforms $P \in S^3$ to $h(P) \in S^2$.

For future applications, we write h in suitable coordinates. Choosing the centre of the stereographic projection appropriately, we get the explicit form of Hopf's map,

$$h(\alpha,\beta,\gamma,\delta) = (\xi,\eta,\zeta) \qquad (25)$$

where

$$\xi = \alpha^2 + \beta^2 + \gamma^2 + \delta^2 \qquad (26)$$

$$\eta = 2 (\alpha \delta + \beta \gamma)$$
(27)

$$\zeta = 2 (\alpha \gamma - \beta \delta)$$
(28)

The last formulas allow us to extend h to all of \mathbb{R}^4 . We shall denote this extension also by h. Thus

h :
$$\mathbb{R}^4 \longrightarrow \mathbb{R}^3$$
 (29)
($\alpha, \beta, \gamma, \delta$) $\longrightarrow (\xi, \eta, \zeta)$

Both descriptions of the Hopf map (with 4 real or with 2 complex coordinates) have their merits:

The former enables one to immediately carry the construction over to maps from S^7 to S^4 and from S^{15} to S^8 . We only have to replace the field R in the definition by the complex numbers C or by the skew-field H of quaternions, respectively, while the latter is more useful for direct calculations. Both advantages, however, can be combined, if we represent the three-sphere S^3 by a single quaternionic coordinate instead of using two complex or four real numbers. This leads to much more compact expressions.

We write the typical quaternion in the form

$$q = a + b i + c j + d k$$
(30)

with the usual basis $\{1, i, j, k\}$ for \mathbb{H} , obeying the defining relations

$$i^2 = j^2 = k^2 = -1$$
 (31)

$$\mathbf{j}\mathbf{k} = \mathbf{i}$$
 $\mathbf{k}\mathbf{i} = \mathbf{j}$ $\mathbf{i}\mathbf{j} = \mathbf{k}$ (32)

$$k j = -i \quad i k = -j \quad j i = -k$$
 (33)

The conjugate quaternion to q is

$$\vec{q} = \mathbf{a} - \mathbf{b} \mathbf{i} - \mathbf{c} \mathbf{j} - \mathbf{d} \mathbf{k}$$
(34)

and the real and imaginary parts of q will be denoted by

$$\operatorname{Re}(q) = \frac{1}{2}(q + \overline{q}) = a$$
 (35)

and

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$$Im(q) = \frac{1}{2}(q - \overline{q}) = b \mathbf{i} + c \mathbf{j} + d \mathbf{k}$$
 (36)

respectively.

The norm of q is the nonnegative real number

$$q \bar{q} = a^2 + b^2 + c^2 + d^2$$
 (37)

which does not vanish except if q = 0, and the (Euclidian) scalar product of two quaternions q and u is

$$\langle q, u \rangle = \operatorname{Re}(q\overline{u}) = \operatorname{Re}(u\overline{q}) = \operatorname{Re}(\overline{q}u) = \operatorname{Re}(\overline{u}q)$$
 (38)

After these preparations, we may write the (standard) three-sphere as the set of quaternions with norm 1,

$$S^{3} = \left\{ u \in \mathbb{H} \mid u \overline{u} = 1 \right\}$$
(39)

while the two-sphere consists of the quaternions with norm 1 and vanishing real part,

$$\mathbf{S}^{2} = \left\{ \mathbf{u} \in \mathbf{H} \mid \mathbf{u} \,\overline{\mathbf{u}} = 1; \, \operatorname{Re}(\mathbf{u}) = 0 \right\}$$
(40)

With this conventions, the (standard) Hopf map (29) is given by the exceedingly simple formula

$$h(u) = u i u$$

We conclude this section with the important

<u>Theorem 1 (Hopf):</u>

The fibres of the Hopf map h (= inverse images of some $x \in S^2$) are great circles on S^3 .

Proof:

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Assume that y and z are in the same fibre,

$$h(y) = h(z) \tag{42}$$

Setting

 $u = y^{-1} z = \overline{y} z$ (43)

(note that the norm of y is 1 !), we obtain

 $y i \overline{y} = h(y) = h(z) = h(yu) = y u i \overline{y}$ (44)

Since y and \overline{y} are invertible, this implies

 $i = u i \overline{u} = u i u^{-1}$ (45)

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which, together with the norm condition, shows that u is of the form

 $u = \cos \varphi + i \sin \varphi \tag{47}$

(41)

for some angle φ . Hence the fibre of h(y) is

$$h^{-1}(h(y)) = \left\{ y \cos \varphi + y i \sin \varphi \right\} .$$
 (48)

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which is indeed a great circle.

We shall apply these known facts about the Hopf fibration in the next section and demonstrate how to regularise the perturbed Kepler problem. It will turn out that the use of quaternions is highly advantageous in comparison to the real or complex form of h.

3. HOPF REGULARISATION

Levi-Cività [1956] generalised the ideas described in section 1 to the twodimensional perturbed Kepler problem. Inspired by methods applied earlier by Hill [1906] and others, he used one complex coordinate

$$w = x + i y \tag{49}$$

instead of the Cartesian $(x, y) \in \mathbb{R}$.

This has the advantage that one can immediately extend the formulas for the linear motion to this case. Here, however, we shall be interested in the three-dimensional analogue, which has been solved for the first time by Kustaanheimo [1964]. His approach, unfortunately, is obscured by the use of real (4,4)-matrices instead of the more natural quaternions. This makes his presentation difficult to read.

This unplesant custom was followed later in the monograph by Stiefel and Scheifele [1971], who even state wrongly that a regularisation of the type in question could not be achieved with the help of quaternions. This is the more surprising as they mention the Hopf fibration explicitly in the appendix to the book. The source of the error seems to be an unsuitable choice of signs in their matrices.

We shall demonstrate in this section that a regularisation can indeed be carried through with the quaternionic form of the Hopf map.

At the same time it will become apparent that this leads to very simple equations of motion, much simpler at least than the matrix version is.

Almost all we have to do is to introduce a parameter space which is connected to the 3-dimensional configuration space \mathbb{R}^3 via a quadratic map (compare this with the situation in the 1-dimensional case !).

For topological reasons (homotopy theory), such a map does not exist if we require the parameter space also to be 3-dimensional. This may explain that the regularisation has not been found earlier.

If we allow the parameter space to be 4-dimensional, the problem totally disappears.

The foregoing discussion suggests to use the Hopf map h introduced earlier to replace the position vector

:

$$\mathbf{x} = (\xi, \eta, \zeta) \tag{50}$$

by a parameter four-vector

$$u = (\alpha, \beta, \gamma, \delta)$$
(51)

We identify x and u with the associated quaternions,

$$\mathbf{x} = \boldsymbol{\xi} \mathbf{i} + \eta \mathbf{j} + \boldsymbol{\zeta} \mathbf{k} \tag{52}$$

and

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$$\mathbf{u} = \boldsymbol{\alpha} + \boldsymbol{\beta} \, \mathbf{i} + \boldsymbol{\gamma} \, \mathbf{j} + \boldsymbol{\delta} \, \mathbf{k} \tag{53}$$

and assume them to be connected by the Hopf map: -

$$\mathbf{x} = \mathbf{h}(\mathbf{u}) \tag{54}$$

We can hope that this Ansatz, together with the introduction of the parametric time τ instead of the coordinate time t, see section 1, will lead to regular equations.

There is, however, a minor obstacle. Since the parameter space is of higher dimension (4) than the configuration space (3), the auxiliary quaternion u is not fixed uniquely for given x. This means that we have to introduce an additional condition to get a closed system of equations.

We saw already that the fibres $h^{-1}(x)$ of the Hopf map are great circles in \mathbb{R}^4 . Thus a rotation of u along this circle will not affect the position x.

The optimal and most natural restriction will be to require that the motion in u-space is everywhere orthogonal to the h-fibres.

This demand is completely equivalent to the so-called "bilinear equation" of Stiefel and Scheifele [1971], but here its geometric interpretation is obvious.

By Hopf's Theorem 1, the fibre passing through $u \neq 0$ is

$$h^{-1}(h(u)) = \left\{ u \cos \varphi + u i \sin \varphi \mid \varphi \in \mathbb{R} \right\}$$
(55)

and (up to a real factor) the tangent vector is u i. The geometric restric-

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tion hence reads

$$0 = 2 \langle \mathbf{u}', \mathbf{u} \mathbf{i} \rangle = -\mathbf{u}' \mathbf{i} \, \overline{\mathbf{u}} + \mathbf{u} \mathbf{i} \, \overline{\mathbf{u}}' \tag{56}$$

or the same with dots instead of the primes. We therefore get the important relation

$$u i \overline{u}' = u' i \overline{u}$$
 (57)

Next, we have to substitute

$$\mathbf{x} = \mathbf{u} \, \mathbf{i} \, \mathbf{\overline{u}} \tag{58}$$

and

;

$$dt = |x| d\tau = \langle u, u \rangle d\tau$$
 (59)

into the equation of motion,

$$\ddot{\mathbf{x}} + \frac{\mu}{|\mathbf{x}|^3} = \operatorname{grad}_{\mathbf{x}} \mathbf{V}(\mathbf{x})$$
(60)

and the energy conservation law,

$$\frac{1}{2} \langle x, x \rangle = \frac{\mu}{|x|} + V(x) + E$$
 (61)

where again the integration constant E is the energy per unit mass of the planet.

We begin with the transformation of the gradient. Note that x and u have been written as row vectors, so the gradient is a column vector. What we really need, however, is the transpose of grad V, because only this can be interpreted as a quaternion.

We insert (58) into V(x) and get V as a function of the parameter u. The connection between the u- and x-gradients is found from the chain rule,

$$\operatorname{grad}_{u} V = \frac{\partial x}{\partial u} \cdot \operatorname{grad}_{x} V = J \cdot \operatorname{grad}_{x} V$$
 (62)

where J is the Jacobi matrix of the Hopf map,

$$J = \frac{\partial x}{\partial u} = \begin{pmatrix} 0 & 2\alpha & 2\delta & 2\gamma \\ 0 & 2\beta & 2\gamma & -2\delta \\ 0 & -2\gamma & 2\beta & 2\alpha \\ 0 & -2\delta & 2\alpha & -2\beta \end{pmatrix}$$
(63)

Though J is singular, formula (62) can be solved for $\operatorname{grad}_{\mathbf{x}} \mathbf{V}$ with the obvious relation

$$J J = 4 \langle u, u \rangle Diag(0, 1, 1, 1)$$
 (64)

We are led to

$$\operatorname{grad}_{x} V = \frac{1}{4} \langle u, u \rangle^{-1} \quad {}^{t} J \cdot \operatorname{grad}_{u} V(u)$$
 (65)

To find the perturbative acceleration, we have to transpose. The result is

with the abbreviation

$$K = \frac{1}{2} t(\operatorname{grad}_{u} V) \cdot J$$
(67)

or, in components,

$$K = (\alpha \partial_{\alpha} V + \beta \partial_{\beta} V - \gamma \partial_{\gamma} V - \delta \partial_{\delta} V) \mathbf{1} + (\delta \partial_{\alpha} V + \gamma \partial_{\beta} V + \beta \partial_{\gamma} V + \alpha \partial_{\delta} V) \mathbf{j} + (\gamma \partial_{\alpha} V - \delta \partial_{\beta} V + \alpha \partial_{\gamma} V - \beta \partial_{\delta} V) \mathbf{k}$$

$$(68)$$

This concludes the required transformation of the force term. The remaining calculations are even easier. By the chain rule, we have

$$x = \langle u, u \rangle^{-1} x'$$
 (69)

and

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$$\ddot{x} = \langle u, u \rangle^{-3} \left\{ \langle u, u \rangle x'' - 2 \langle u, u' \rangle x' \right\}$$
(70)

On the other hand, differentiating the Hopf map and applying the geometric by-condition (57) provides us with

$$\mathbf{x}' = 2 \mathbf{u}' \mathbf{i} \, \overline{\mathbf{u}} \tag{71}$$

as well as

$$\mathbf{x}'' = 2 \mathbf{u}'' \mathbf{i} \, \overline{\mathbf{u}} + 2 \mathbf{u}' \mathbf{i} \, \overline{\mathbf{u}}' \tag{72}$$

We collect the results. The energy condition is in the parametric form

$$2 < u', u' > = \mu + (V + E) < u, u >$$
 (73)

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and the equation of motion itself is

$$2 < u, u > u'' i \overline{u}' + 2 < u, u > u' i \overline{u}' - 4 < u, u' > u' i \overline{u} + \mu u i \overline{u} =$$

$$= \frac{1}{2} K < u, u >^{2}$$
(74)

A slight rearrangement using the identity

$$2 \langle u, u' \rangle u' i \overline{u} = (u \overline{u}' + u' \overline{u}) u' i \overline{u}' =$$

$$= \langle u', u' \rangle u i \overline{u} + \langle u, u' \rangle u' i \overline{u}$$
(75)

reduces the last formula to

2 u" i
$$\overline{u}$$
 - $\{2 < u', u'> -\mu\}$ u i \overline{u} = $\frac{1}{2} K < u, u>^2$ (76)

We next insert the energy equation and divide by $\langle u, u \rangle$,

$$2 u'' i \overline{u} = (V + E) u i \overline{u} + \frac{1}{2} K < u, u >$$
 (77)

Finally, we obtain after a further simplification the explicit version of the quaternionic equation of motion,

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(78)

$$2 u'' = (V + E) u - \frac{1}{2} K u i$$

This is obviously completely regular, as desired.

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