

GEOMETRY OF SPINOR REGULARIZATION

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Abstract. The Kustaanheimo theory of spinor regularization is given a new formulation in terms of geometric algebra. The Kustaanheimo–Stiefel matrix and its subsidiary condition are put in a spinor form directly related to the geometry of the orbit in physical space. A physically significant alternative to the KS subsidiary condition is discussed. Derivations are carried out without using coordinates.

The spinor regularization of the Kepler motion by Kustaanheimo (1964) was given a matrix formulation by Kustaanheimo and Steifel (1965). This matrix formulation has been developed as a general computational method by Stiefel and Scheifele (1971). In spite of its theoretical and computational advantages, the method has not been widely employed in astrodynamics and celestial mechanics. This may be because the method appears to be founded on an *ad hoc* mathematical trick of obscure significance. We believe that this mistaken impression is the result of using an inappropriate matrix formulation. We give here an alternative formulation which reveals a clear and simple geometric foundation for the method.

The theory will be reformulated here in terms of *geometric algebra*. The fundamentals of geometric algebra are developed in Hestenes (1971) and Hestenes (1983). We shall employ the basic definitions, notations and results given there, so the reader is advised to become familiar with one of these references before proceeding. The reasons for using geometric algebra should be reiterated here, however. It suffices to note that geometric algebra integrates quaternion algebra and conventional vector algebra into a single system combining the advantages of both algebras considered separately. In particular, it enables us to define vectors and spinors and perform computations without breaking them into components. The advantage of this is most obvious in the representation of rotations.

Geometric algebra enables us to write any rotation-dilation of Euclidean 3-space in the canonical form

$$\mathbf{x}' = U^\dagger \mathbf{x} U, \tag{1}$$

where \mathbf{x} and \mathbf{x}' are vectors and U is a quaternion with conjugate U^\dagger . This equation

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describes the rotation and dilation of any given vector \mathbf{x} into a unique vector \mathbf{x}' . A quaternion U which is used in this way to describe a rotation-dilation may be called a *spinor*, because it is mathematically equivalent to the spinors used in quantum mechanics (Hestenes and Gurtler, 1971; Hestenes, 1979). One might refer to U as the *quaternion form* (or representation) of a spinor, to distinguish it from the *matrix representation* of a spinor commonly used in quantum mechanics or the one employed by Kustaanheimo (1964).

The modulus $|U|$ of the spinor U is a positive scalar determined by

$$|U|^2 = U^\dagger U = U U^\dagger.$$

Consequently, the spinor U , like any nonzero quaternion, has an inverse

$$U^{-1} = |U|^{-2} U^\dagger.$$

Equation (1) can now be written in the form

$$\mathbf{x}' = |U|^2 (U^{-1} \mathbf{x} U).$$

This exhibits the transformation as the composite of a rotation $U^{-1} \mathbf{x} U$ and a dilation by a scale factor $|U|^2$. A proof that any rotation can be put in the form $U^{-1} \mathbf{x} U$ is given, for example, in Hestenes (1971). Of greatest importance is the fact that this representation of a rotation is completely coordinate-free.

1. Position Vector and Spinor

Let \mathbf{r} be the radius vector between two particles, or, as a special case, the position of a single particle relative to a fixed center of force. In either case we shall refer to \mathbf{r} as the *position* of a particle.

The position \mathbf{r} relative to a *fixed* unit vector σ_1 is determined by a spinor U in the equation

$$\mathbf{r} = U^\dagger \sigma_1 U. \quad (2)$$

This is just Equation (1) applied to a single vector rather than regarded as a linear transformation of the whole vector space. Squaring (2), we get $r^2 = |U|^4$, so

$$r = |\mathbf{r}| = |U|^2. \quad (3)$$

Thus, the radial distance r is represented as the scale factor $|U|^2$ of a rotation-dilation.

Given \mathbf{r} , the corresponding spinor U is not uniquely determined by (2). Indeed, if S is a spinor such that

$$S^\dagger \sigma_1 S = \sigma_1, \quad (4)$$

then (2) gives us

$$\mathbf{r} = U^\dagger \sigma_1 U = V^\dagger \sigma_1 V, \quad (5)$$

where

$$V = SU, \quad (6)$$

and S is arbitrary except for the condition (4). The condition (4) simply states that σ_1 is an eigenvector of the rotation $S^\dagger \mathbf{x} S$. In other words, S may be any spinor describing a rotation about the σ_1 axis. From Hestenes (1971) or Hestenes (1983), we know that such a spinor can be written in the parametric form

$$S = e^{(1/2)i\sigma_1\phi}, \quad (7)$$

where ϕ is the scalar angle of rotation and i is the unit pseudoscalar. For the purposes of this paper, the only thing one needs to know about i are that i commutes with all vectors and $i^2 = -1$.

Let us refer to the transformation (6) of U into V as a *gauge transformation*, because it is similar to the gauge transformation of a spinor state function in quantum theory. We say then that Equation (2) is invariant under the one-parameter group of gauge transformations specified by (6) and (4) or (7). If Equation (2) is regarded as a linear transformation of the vector σ_1 into \mathbf{r} , the *gauge invariance* simply means that this transformation is invariant under a rotation about the radial axis. We suppose that σ_1 is some definite unit vector, though the choice is arbitrary. Given σ_1 , by Equation (2) a spinor U determines a unique vector \mathbf{r} , but the vector \mathbf{r} , determines U only up to a gauge transformation. This nonunique correspondence between spinors and vectors is to be expected, of course, because it takes four scalar parameters to specify the quaternion U but only 3 parameters to specify the vector \mathbf{r} . To associate a unique spinor U with the vector \mathbf{r} , we must impose some *gauge condition* consistent with (2) to fix the *gauge* uniquely. A natural gauge condition appears when we consider kinematics.

2. Vector and Spinor Velocity

Let $\mathbf{r} = \mathbf{r}(t)$ be the orbit of a particle in *position space*. The *position* r and *velocity* $\dot{\mathbf{r}} = d\mathbf{r}/dt$ determine the *angular momentum* (per unit mass)

$$\mathbf{h} = \mathbf{r} \times \dot{\mathbf{r}}. \quad (8)$$

As defined in Hestenes (1971 and 1983), the geometric product of vectors \mathbf{r} and $\dot{\mathbf{r}}$ are related to the dot and cross products of conventional vector calculus by

$$\mathbf{r}\dot{\mathbf{r}} = \mathbf{r} \cdot \dot{\mathbf{r}} + i(\mathbf{r} \times \dot{\mathbf{r}}) = r\dot{r} + i\mathbf{h}. \quad (9)$$

The kinematic significance of this quantity will become apparent in the following.

Equation (2) relates an orbit $U = U(t)$ in *spinor space* to an orbit $\mathbf{r} = \mathbf{r}(t)$ in *position space*. We still need to relate the velocity \dot{U} in spinor space to the velocity $\dot{\mathbf{r}}$ in position space. Differentiating $r = |U|^2$, we obtain

$$\dot{r} = \dot{U}U^\dagger + U\dot{U}^\dagger = 2\langle \dot{U}U^\dagger \rangle, \quad (10)$$

where $\langle Q \rangle$ means *scalar part* of Q . Next, it will be convenient to introduce a quaternion W defined by

$$W = 2U^{-1}\dot{U} = 2r^{-1}U^\dagger\dot{U} = r^{-1}\dot{\mathbf{r}} + i\boldsymbol{\omega}, \quad (11)$$

where $\boldsymbol{\omega}$ is a vector and (10) has been used to determine that $\langle W \rangle = r^{-1}\dot{\mathbf{r}}$.

We can put (11) in the form

$$\dot{U} = \frac{1}{2}UW, \quad (12)$$

from which we obtain $\dot{U}^\dagger = \frac{1}{2}W^\dagger U^\dagger$. If we insert these expressions into the equation

$$\dot{\mathbf{r}} = \dot{U}^\dagger \boldsymbol{\sigma}_1 U + U^\dagger \boldsymbol{\sigma}_1 \dot{U}$$

obtained by differentiating (2), we get

$$\dot{\mathbf{r}} = \frac{1}{2}(W^\dagger \mathbf{r} + \mathbf{r}W). \quad (13)$$

Using (11) this can be written

$$\dot{\mathbf{r}} = \dot{\mathbf{r}}\hat{\mathbf{r}} + \frac{1}{2}i(\mathbf{r}\boldsymbol{\omega} - \boldsymbol{\omega}\mathbf{r}).$$

Then using $\mathbf{r}\boldsymbol{\omega} = \mathbf{r} \cdot \boldsymbol{\omega} + i(\mathbf{r} \times \boldsymbol{\omega})$, we obtain

$$\dot{\mathbf{r}} = \dot{\mathbf{r}}\hat{\mathbf{r}} + \boldsymbol{\omega} \times \mathbf{r}. \quad (14)$$

Thus, we identify $\boldsymbol{\omega}$ as the *angular velocity* of the orbit $\mathbf{r} = \mathbf{r}(t)$.

According to (14), the radial component of $\boldsymbol{\omega}$ is irrelevant to $\dot{\mathbf{r}}$. Hence, we are free to eliminate it by introducing the *subsidiary condition*

$$\boldsymbol{\omega} \cdot \mathbf{r} = \langle \boldsymbol{\omega}\mathbf{r} \rangle = 0. \quad (15)$$

This condition can be written in several equivalent ways; thus,

$$\boldsymbol{\omega}\mathbf{r} = -\mathbf{r}\boldsymbol{\omega}$$

or,

$$W^\dagger \mathbf{r} = \mathbf{r}W, \quad (16)$$

which after inserting (11) and (2), gives us

$$\dot{U}^\dagger \boldsymbol{\sigma}_1 U = U^\dagger \boldsymbol{\sigma}_1 \dot{U}. \quad (17)$$

This is equivalent to the scalar condition

$$\langle iU^\dagger \boldsymbol{\sigma}_1 \dot{U} \rangle = \langle i\boldsymbol{\sigma}_1 \dot{U}U^\dagger \rangle = 0. \quad (18)$$

Thus, we have expressed the subsidiary condition as a relation between U and its derivative \dot{U} . By expressing U and \dot{U} in terms of components, one can show that (18) is equivalent to the matrix form of the KS subsidiary condition.

Now, using (16) in (13) we obtain

$$\dot{\mathbf{r}} = \mathbf{r}W.$$

Solving for W and using (11), we get the fundamental result

$$W = 2U^{-1}\dot{U} = \mathbf{r}^{-1}\dot{\mathbf{r}} = r^{-1}\dot{r} + i\boldsymbol{\omega}. \quad (19)$$

Comparison with (9) shows us that the angular velocity is related to the angular momentum by

$$\boldsymbol{\omega} = r^{-2}\mathbf{h}.$$

This is a consequence of or, if you prefer, an alternative form of the subsidiary condition (15).

Equation (19) specifies completely our desired relation between \dot{U} and $\dot{\mathbf{r}}$. Various special relations between \dot{U} and $\dot{\mathbf{r}}$ are easily derived from it. For example,

$$|W|^2 = WW^\dagger = \frac{4}{r}|\dot{U}|^2 = \frac{\dot{\mathbf{r}}^2}{r^2}. \quad (20)$$

Useful alternative forms of (19) are obtained by multiplying it by \mathbf{r} and using (2). Thus, we obtain

$$\dot{\mathbf{r}} = 2U^\dagger\boldsymbol{\sigma}_1\dot{U}, \quad (21)$$

or, equivalently,

$$2r\dot{U} = \boldsymbol{\sigma}_1U\dot{\mathbf{r}}. \quad (22)$$

The KS subsidiary condition is a gauge condition. To see how it determines the gauge, consider an arbitrary time dependent gauge transformation $V = SU$. We wish to relate \dot{V} to \dot{U} to determine the effect of the gauge transformation. Differentiating (7) with $\phi = \phi(t)$, we have

$$\dot{S} = \frac{1}{2}i\boldsymbol{\sigma}_1\dot{\phi}S = S\frac{1}{2}i\boldsymbol{\sigma}_1\dot{\phi}. \quad (23)$$

So, using (12), we have

$$\dot{V} = \dot{S}U + S\dot{U} = \frac{1}{2}(i\boldsymbol{\sigma}_1\dot{\phi}V + VW).$$

With the help of (5) we can put this in the form

$$\dot{V} = \frac{1}{2}V(i\hat{\mathbf{r}}\dot{\phi} + W). \quad (24)$$

This is a completely general relation showing how W can be altered by a gauge transformation. Using the specific from (19) for W , we obtain

$$2V^{-1}\dot{V} = 2U^{-1}\dot{U} + i\hat{\mathbf{r}}\dot{\phi} = r^{-1}\dot{r} + i(r^{-2}\mathbf{h} + \hat{\mathbf{r}}\dot{\phi}). \quad (25)$$

This shows explicitly that the gauge transformation adds a radial component $\hat{\mathbf{r}}\dot{\phi}$ to the angular velocity. We can solve (25) for $\dot{\phi}$, with the result

$$\dot{\phi} = -\langle i\hat{\mathbf{r}}2V^{-1}\dot{V} \rangle = -\frac{2}{r}\langle iV^\dagger\boldsymbol{\sigma}_1\dot{V} \rangle. \quad (26)$$

This reduces to the KS subsidiary condition (18) if and only if $\dot{\phi} = 0$. Thus, the KS condition fixes the gauge to a constant value. In other words, the gauge can be chosen freely at one time, but its value for all other times is then fixed by the KS condition.

We have proved that any alternative to the KS gauge condition will have in general, an angular velocity with a nonvanishing radial component. Equation (14) shows that a radial component of the angular velocity will not affect the velocity $\dot{\mathbf{r}}$ in position space, so we are free to adopt alternative gauge conditions. A physically significant alternative will be discussed in Section 4. In the meantime, we stick with the KS condition.

3. The Spinor Equation of Motion

The spinor equation of motion corresponding to a given equation of motion in position space is most easily found by differentiating (22). Thus,

$$\begin{aligned} 2\frac{d}{dt}(r\dot{U}) &= \sigma_1 U\ddot{\mathbf{r}} + \sigma_1 \dot{U}\dot{\mathbf{r}} \\ &= UU^{-1}\sigma_1 U\ddot{\mathbf{r}} + \sigma_1 \left(\frac{\sigma_1 U\dot{\mathbf{r}}}{2r}\right)\dot{\mathbf{r}}. \end{aligned}$$

Hence,

$$2\frac{d^2U}{ds^2} = U(\mathbf{r}\ddot{\mathbf{r}} + \frac{1}{2}\dot{\mathbf{r}}^2), \quad (27)$$

where $d/ds = rd/dt$. This is *the fundamental equation* determining the relation between vector and spinor equations of motion.

Given the vector equation of motion

$$\ddot{\mathbf{r}} = -\mu\frac{\mathbf{r}}{r^3} + \mathbf{f}, \quad (28)$$

where \mathbf{f} is an arbitrary perturbing force (per unit mass), the spinor equation of motion is obtained by substitution into (27). Thus, we obtain

$$2\frac{d^2U}{ds^2} - EU = U\mathbf{r}\mathbf{f} (= r\sigma_1 U\mathbf{f}), \quad (29)$$

where E is the Kepler energy

$$E = \frac{1}{2}\dot{\mathbf{r}}^2 - \frac{\mu}{r} = |U|^{-2} \left(2\left|\frac{dU}{ds}\right|^2 - \mu \right). \quad (30)$$

Equation (29) is the KS equation in terms of geometric algebra. It becomes a determinate equation in spinor space when \mathbf{f} is given as an explicit function of \mathbf{r} and $\dot{\mathbf{r}}$ so $\mathbf{r}\mathbf{f}$ can be expressed as a function of U and \dot{U} by using (2) and (21).

Note that the perturbation factor $\mathbf{r}\mathbf{f} = \mathbf{r}\cdot\mathbf{f} + i(\mathbf{r}\times\mathbf{f})$ in (29) decomposes naturally into a radial part $\mathbf{r}\cdot\mathbf{f}$ which can alter the size and shape of the osculating Kepler orbit and a torque $i(\mathbf{r}\times\mathbf{f})$ which can alter the attitude (or orientation) of the orbit in space. This is closely related to the alternative gauge condition discussed in the next section.

4. An Alternative Gauge Condition

We have seen that the KS spinor state function U is related to any acceptable alternative state function V by a gauge transformation $V = SU$. According to (5), U and V determine the same orbit $\mathbf{r} = \mathbf{r}(t)$. As a geometrically significant alternative to the KS gauge condition, consider

$$V^{-1}\sigma_3V = \hat{\mathbf{h}} = h^{-1}\mathbf{h}, \quad (31)$$

where σ_3 is an arbitrarily chosen fixed unit vector orthogonal to σ_1 . Equation (31) is consistent with (5) since $\mathbf{h}\cdot\mathbf{r} = 0$. Therefore it is acceptable as a gauge condition.

The condition (31) has a number of advantages. To begin with, it assures that V has a direct geometrical interpretation. The spinor V determines both the position \mathbf{r} by (5) and the plane of motion in position space by (31). Conversely, given the position \mathbf{r} and the plane of motion specified by \mathbf{h} , then V is determined uniquely (except for sign) by Equations (5) and (31). Thus, V provides a unique and direct description of the position and plane of motion at every time.

A further advantage of using V appears when we relate it to the spinor R which determines the *Kepler frame*

$$\mathbf{e}_k = R^\dagger\sigma_kR \quad (32)$$

($k = 1, 2, 3$). This frame, with $\sigma_2 = \sigma_3 \times \sigma_1$, is specified by the physical conditions

$$\mathbf{e}_3 = R^\dagger\sigma_3R = \hat{\mathbf{h}} \quad (33)$$

and

$$\mathbf{e}_1 = R^\dagger\sigma_1R = \hat{\boldsymbol{\varepsilon}}, \quad (34)$$

where $\boldsymbol{\varepsilon}$ is the eccentricity vector pointing towards periapse of the osculating orbit.

Equations (31), (33), and (34) determine a unique factorization of the *spinor state function* V into

$$V = ZR, \quad (35)$$

where Z and R can be regarded as ‘internal’ and ‘external’ state functions respectively. Consistency of (31) with (33) implies that

$$Z^\dagger\sigma_3Z = r\sigma_3.$$

Hence, we can write Z in the form

$$Z = (re^{i\sigma_3\theta})^{1/2}. \quad (36)$$

Then, using (31) and (34) we obtain

$$\mathbf{r} = V^\dagger \boldsymbol{\sigma}_1 V = R^\dagger \boldsymbol{\sigma}_1 Z^2 R = r \hat{\boldsymbol{\varepsilon}} e^{i\hat{\mathbf{h}}\theta}. \quad (37)$$

This exhibits θ as the *true anomaly* of the osculating orbit.

The *internal state function* Z describes the size and shape of the osculating orbit as well as location on the orbit. If we take the eccentricity $\varepsilon = |\boldsymbol{\varepsilon}|$, the angular momentum $h = |\mathbf{h}|$, and the true anomaly θ as internal state variables, then Z is a determinate function $Z = Z(\varepsilon, h, \theta)$ of these variables. The algebraic form of Z exhibited in (36) shows that we can identify Z with the Levi–Civita function (Stiefel and Scheifele, 1971), where the constant bivector $i\boldsymbol{\sigma}_3 = \boldsymbol{\sigma}_1 \boldsymbol{\sigma}_2$ plays the role of the unit imaginary satisfying $(i\boldsymbol{\sigma}_3)^2 = -1$.

Although the fixed reference frame $\{\boldsymbol{\sigma}_k\}$ can be chosen arbitrarily, it will most often be convenient to associate it with an initial osculating orbit of the particle. For Kepler motion the best choice is

$$\boldsymbol{\sigma}_1 = \hat{\boldsymbol{\varepsilon}}_0 \quad \text{and} \quad \boldsymbol{\sigma}_3 = \hat{\mathbf{h}}, \quad (38)$$

where \mathbf{h}_0 is the initial angular momentum and $\boldsymbol{\varepsilon}_0$ is the initial eccentricity vector. The initial value of the spinor V is then

$$V_0 = Z_0 = (\hat{\boldsymbol{\varepsilon}}_0 \mathbf{r}_0)^{1/2} = r_0^{1/2} e^{(1/2)i\boldsymbol{\sigma}_3\theta_0}, \quad (39)$$

where θ_0 is the initial true anomaly.

The *external state function* R determines the attitude of the osculating orbit in position space. A first order equation of motion for R has been derived and discussed in Hestenes (1983).

The factorization $V = ZR$ should be of value in perturbation theory, because it admits a systematic separation of perturbation effects determined by the geometry of the orbital elements. Unfortunately, the KS Equation (29) loses its simplicity when translated into an equation for V instead of U . Although, of course, V can be identified with U in the absence of perturbations. On the other hand, if the factorization $V = ZR$ is used, it might be best to work with a pair of weakly coupled equations for R and Z , but we will not pursue that theme here.

5. Discussion

The advantages of formulating KS theory in terms of geometric algebra instead of matrix algebra should be evident. First, geometric algebra enables us to formulate the entire theory and perform all necessary manipulations without decomposing the spinor state function or any other quantity into components. Second, the spinor state function and its derivative have definite geometric interpretations characterizing the geometry of an orbit in physical space. Consequently, we were able to identify the elementary kinematical meaning of the subsidiary condition (18) which is not at all evident in the matrix formulation. Indeed, this important point seems to have been overlooked in all previous treatments of KS theory.

Our formulation makes it clear that the transformation of the Newtonian equation of motion into a spinor equation of motion is a *general method*, not a special method concerned only with regularization and perturbations of Kepler motion, as one might think from the matrix formulation Stiefel and Scheifele (1971). Thus, our development of the theory up to key Equation (27) is completely general. It is interesting to note that the usual regularizing change in the time variable is perfectly natural in this equation, though no issue of regularization can be raised until the dynamics is introduced. We introduce dynamics into that equation in a single step, and the Newtonian (or Coulomb) interaction is automatically regularized. Nevertheless, the method should be useful for treating other interactions as well.

It is also interesting to note that our spinor representation of an ‘orbital state’ in classical mechanics is closely related to the spinor representation of a particle state in quantum mechanics. The quaternion form for a spinor is used for the wave function of an electron in Hestenes (1971 and 1983). Remarkably, the electron spin is determined by the electron wave function in the same way that the angular momentum vector is determined by our ‘classical’ spinor state function V in Equation (27). This suggests new possibilities for interrelating the methods of classical and quantum mechanics.

A representation of KS theory in terms of quaternion algebra has been developed by Velte (1978). His quaternion state function is essentially the same as ours. However, his method of deriving the quaternion equation of motion does not work if perturbations to Kepler motion are included. Consequently, he also fails to notice the kinematical basis of the KS subsidiary condition. The quaternions form a subalgebra of geometric algebra, but quaternion algebra by itself is not a satisfactory substitute for geometric algebra, because it fails to distinguish between vectors and bivectors. This essential point is discussed in Hestenes (1971).

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