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Abstract. It is shown that the Kustaanheimo–Stiefel transformation which transforms the three-dimensional Kepler problem into that for a four-dimensional harmonic oscillator may be expressed in terms of quaternions. In this form the transformation represents a continuous mapping of a triad of orthonormal vectors fixed in space into a rotating triad of orthogonal vectors where one of the unit vectors is mapped into the position vector of a moving particle. The reduction of the Kepler problem to that of a harmonic oscillator is straightforward and direct in the quaternion formalism. The complex stereographic transformation used recently by the author in the corresponding reduction of Schrödinger's equation for the hydrogen atom is shown to be closely related to the quaternion representation.

1. Introduction

The KS transformation was introduced by Kustaanheimo and Stiefel (1965) as a means of obtaining equations for the classical Kepler problem which are regular at the centre of attraction. This has particular advantages in the numerical calculation of perturbed motions (see Stiefel and Scheifele 1971). The KS transformation maps the three-dimensional (3D) space of a Kepler orbit into a 4D space in which the equation of motion becomes that of a harmonic oscillator with constraint. The transformation also has applications in the corresponding quantum mechanical problem and was used by Ho and Inomata (1982) in the calculation of the Coulomb Green function using the Feynman path integral method following earlier work by Duru and Kleinert (1979).

In the present paper we show that the KS transformation may be expressed in terms of quaternions and that in this form it has a simple kinematical interpretation. The use of quaternions seems particularly apt although the closely related Pauli spin matrices could readily be used instead. We also show that the quaternion formalism has the further advantage that the reduction of the Kepler problem to the 4D harmonic oscillator may be made in a direct way in contrast to the indirect approach used by Kustaanheimo and Stiefel (1965) and by Stiefel and Scheifele (1971) in their formalism.

In § 2 we give a brief description of the 2D Kepler problem and its reduction to the 2D harmonic oscillator, followed in § 3 by a summary of the main features of the KS transformation for the 3D case. Expressed in terms of quaternions we show in § 4 that the KS transformation may be interpreted as a transformation which maps continuously a triad of orthonormal vectors fixed in space into a rotating triad of orthogonal vectors in such a way that one of the unit vectors is mapped into the position vector of a moving particle. The four variables involved in the KS transformation correspond to the four components of a quaternion and are determined by the three angles needed to specify the rotation of the triad of vectors as a rigid system and by the length of the position vector of the particle which determines an expansion. The arbitrariness of the component of rotation about the position vector of the particle leads naturally to the constraint condition which forms part of the KS transformation and reduces the number of degrees of freedom from four to three.

In § 5 it is shown that the reduction of the Kepler problem in 3D to the 4D harmonic oscillator may be achieved in a direct manner using the quaternion formalism. Expressions are also obtained for the angular momentum of the Kepler orbit in terms of the six constant components of the angular momentum of the harmonic oscillator. It is also shown that the KS transformation expressed in terms of quaternions is closely related to the complex stereographic transformation used by Cornish (1984) to transform Schrödinger's equation for the hydrogen atom into the wave equation for two coupled 2D harmonic oscillators.

2. The two-dimensional case

In 2D the equation of motion for a particle of mass m moving under an inverse square law force of attraction towards the origin may be expressed as

$$m\ddot{\xi} = -\kappa^2|\xi|^{-3}\xi, \tag{1}$$

where $\xi = x_1 + \mathrm{i}x_2$. The conserved energy E and angular momentum L are given by

$$E = \tfrac{1}{2}m|\dot{\xi}|^2 - \kappa^2|\xi|^{-1}, \qquad 2\mathrm{i}L = m(\xi^*\dot{\xi} - \xi\dot{\xi}^*), \tag{2}$$

where * denotes the complex conjugate. Make the substitution

$$\xi = \zeta^2, \qquad \zeta = v_1 + \mathrm{i}v_2, \tag{3}$$

which is equivalent to

$$x_1 = v_1^2 - v_2^2, \qquad x_2 = 2v_1v_2, \tag{4}$$

so that v_1 and v_2 are plane parabolic coordinates, and replace the time t by a new independent variable s defined by

$$\mathrm{d}s/\mathrm{d}t = |\xi|^{-1} = |\zeta|^{-2}. \tag{5}$$

Then equations (1) and (2) reduce to

$$\zeta'' = (E/2m)\zeta, \tag{6}$$

$$\kappa^2 = 2m|\zeta'|^2 - E|\zeta|^2, \qquad \mathrm{i}L = m(\zeta^*\zeta' - \zeta\zeta^{*\prime}), \tag{7}$$

where $'$ denotes the derivative with respect to s. In the case of bounded Kepler orbits in the ξ plane $E<0$, and the corresponding motion in the ζ plane is that of a 2D harmonic oscillator with frequency $\omega = (-E/2m)^{1/2}$, angular momentum $\frac{1}{2}L$ and energy $\frac{1}{4}\kappa^2$ (the numerical factors occurring in these expressions may be altered by introducing a numerical factor into the definition (5) of s).

The appropriateness of the transformation $\xi = \zeta^2$ arises from the fact that ellipses centred at the origin in the ζ plane are mapped into ellipses with focus at the origin in the ξ plane (see Stiefel and Scheifele 1971). The transformation (4) may also be expressed in matrix form

$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} v_1 & -v_2 \\ v_2 & v_1 \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}. \tag{8}$$

The change of independent variable from t to s leads to an expression for the angular momentum in the ζ plane which has the same form as that in the ξ plane, and also reduces the equation of motion in the ζ plane to that of a harmonic oscillator.

3. The three-dimensional case

Kustaanheimo and Stiefel have shown that the 3D Kepler problem may be reduced to that of a 4D harmonic oscillator by using a transformation to a 4D space given in matrix form by

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ 0 \end{pmatrix} = \begin{pmatrix} u_1 & -u_2 & -u_3 & u_4 \\ u_2 & u_1 & -u_4 & -u_3 \\ u_3 & u_4 & u_1 & u_2 \\ u_4 & -u_3 & u_2 & -u_1 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix}, \tag{9}$$

or more explicitly by

$$x_1 = u_1^2 - u_2^2 - u_3^2 + u_4^2, \qquad x_2 = 2(u_1 u_2 - u_3 u_4), \qquad x_3 = 2(u_1 u_3 + u_2 u_4), \tag{10}$$

where x_1, x_2, x_3 are the cartesian components of the position vector $\boldsymbol{x}$. The time t is replaced by s defined by

$$\mathrm{d}s/\mathrm{d}t = |\boldsymbol{x}|^{-1} = |u|^{-2}, \tag{11}$$

where

$$|\boldsymbol{x}| = (x_1^2 + x_2^2 + x_3^2)^{1/2}, \qquad |u| = (u_1^2 + u_2^2 + u_3^2 + u_4^2)^{1/2}. \tag{12}$$

Then the equation of motion

$$m\ddot{\boldsymbol{x}} = -\kappa^2 |\boldsymbol{x}|^{-3} \boldsymbol{x} \tag{13}$$

is shown to be equivalent in u space to the equations

$$u_\alpha'' = (E/2m) u_\alpha, \qquad \alpha = 1, 2, 3, 4, \tag{14}$$

where E is the total energy of the Kepler orbit and where a prime denotes the derivative with respect to s, provided the parameters u_α satisfy the condition

$$u_4 u_1' - u_3 u_2' + u_2 u_3' - u_1 u_4' = 0. \tag{15}$$

It follows that when $E < 0$ closed orbits in x space correspond by (14) to the motion of a 4D harmonic oscillator in u space of frequency $\omega = (-E/2m)^{1/2}$ subject to the constraint condition (15). The constraint shows that the 4D harmonic oscillator may be regarded as two 2D harmonic oscillators in the 23 and 14 planes coupled in such a way that their angular momenta are equal. It is easily seen that the constraint is consistent with the equation of motion (14) in that if it is satisfied at one value of s then it is satisfied for all s. Many algebraic and geometric properties of the KS transformation are discussed by Stiefel and Scheifele (1971).

4. The KS transformation expressed in terms of quaternions

A quaternion q is expressed in terms of its components q_α ($\alpha = 1$ to 4) by

$$q = q_1 e_1 + q_2 e_2 + q_3 e_3 + q_4 \tag{16}$$

where e_1, e_2, e_3 are unit quaternions which satisfy the relations

$$e_1^2 = -1 = e_2^2 = e_3^2, \qquad e_1 e_2 = e_3 = -e_2 e_1. \tag{17}$$

We shall need to consider only quaternions with real components q_α. A quaternion q is said to be real if $q_1 = 0 = q_2 = q_3$, and imaginary if $q_4 = 0$. The quaternion $\bar{q}$ conjugate to q is defined by

$$\bar{q} = -q_1 e_1 - q_2 e_2 - q_3 e_3 + q_4. \tag{18}$$

Note that

$$q\bar{q} = q_1^2 + q_2^2 + q_3^2 + q_4^2 = |q|^2, \tag{19}$$

and that if p and q are any two quaternions

$$\overline{pq} = \bar{q}\bar{p}. \tag{20}$$

A vector $\boldsymbol{x}$ is conveniently expressed as an imaginary quaternion

$$\boldsymbol{x} = x_1 e_1 + x_2 e_2 + x_3 e_3. \tag{21}$$

If $\boldsymbol{x}$ and $\boldsymbol{y}$ are two vectors in three-space then their product as quaternions may be expressed in terms of their scalar and vector products:

$$\boldsymbol{xy} = -\boldsymbol{x} \cdot \boldsymbol{y} + \boldsymbol{x} \times \boldsymbol{y}. \tag{22}$$

This leads to two useful results

$$\boldsymbol{xy} + \boldsymbol{yx} = -2\boldsymbol{x} \cdot \boldsymbol{y}, \qquad \boldsymbol{xy} - \boldsymbol{yx} = 2\boldsymbol{x} \times \boldsymbol{y}. \tag{23}$$

Quaternions are particularly useful in dealing with rotations in three-space. Thus if q is any unit quaternion, so that $q\bar{q} = 1$, then the transformation $\boldsymbol{x} \to \boldsymbol{y}$ given by

$$\boldsymbol{y} = \bar{q}\boldsymbol{x}q \tag{24}$$

represents a rotation in three-space. Writing

$$q = \cos \tfrac{1}{2}\psi - \sin \tfrac{1}{2}\psi \boldsymbol{n} = \exp(-\boldsymbol{n}\psi/2), \tag{25}$$

where $\boldsymbol{n}$ is a unit imaginary quaternion so that $\boldsymbol{n} \cdot \boldsymbol{n} = -\boldsymbol{nn} = 1$, then $\boldsymbol{y}$ given by (24) is obtained by rotating $\boldsymbol{x}$ about the unit vector $\boldsymbol{n}$ through the angle ψ in the right-hand sense.

Now consider the position vector $\boldsymbol{x}(t)$ of a moving particle. A quaternion $u(t)$ may always be found so that

$$\boldsymbol{x}(t) = \bar{u}(t)e_1 u(t). \tag{26}$$

Writing $|\boldsymbol{x}| = r$, it follows from this that

$$r^2 = \boldsymbol{x}\bar{\boldsymbol{x}} = \bar{u}e_1 u\bar{u}(-e_1)u = |u|^4. \tag{27}$$

In fact (26) represents a transformation whereby the unit vector along the Ox_1 axis undergoes a rotation given by the quaternion $r^{-1/2}u$ to align it with $\boldsymbol{x}$ together with an expansion of length by the factor r. Clearly $u(t)$ at any instant lacks uniqueness to the extent of an arbitrary rotation about $x(t)$. For example, introducing spherical polar angles θ, ϕ so that

$$x = r\cos\theta\, e_1 + r\sin\theta\cos\phi\, e_2 + r\sin\theta\sin\phi\, e_3, \tag{28}$$

a possible choice for u would be

$$u = r^{1/2}\exp(-\tfrac{1}{2}\psi e_1)\exp(-\tfrac{1}{2}\theta e_3)\exp(-\tfrac{1}{2}\phi e_1). \tag{29}$$

Then $r^{-1/2}u$ represents an arbitrary rotation ψ about the Ox_1 axis, followed by a rotation θ about the Ox_3 axis, followed finally by a rotation ϕ about the Ox_1 axis.

The effect of the rotation described by the quaternion $r^{-1/2}u$ on the three unit vectors directed along the coordinate axes of x space may be expressed in terms of a transformation from the set of unit imaginary quaternions e_k to a new set f_k given by

$$rf_k = \bar{u}(t)e_k u(t), \qquad k = 1, 2, 3. \tag{30}$$

The f_k satisfy the same relations (17) as e_k do. f_1, f_2 and f_3 correspond to an orthonormal set of unit vectors which follow the motion in the sense that f_1 is always directed along $x(t)$. The rate of rotation $\Omega(t)$ of this set about $x(t)$ is given by

$$r^2\Omega(t) = r^2\dot{f}_2\cdot f_3 = rf_3\cdot(\mathrm{d}/\mathrm{d}t)(rf_2). \tag{31}$$

Using (30) and (23), and after some algebra, this gives

$$r\Omega(t) = \bar{u}e_1\dot{u} - \dot{\bar{u}}e_1 u. \tag{32}$$

With the choice given by (29) for u, this gives

$$\Omega(t) = \dot{\psi} + \dot{\phi}\cos\theta. \tag{33}$$

When the quaternion u is expressed in terms of its components

$$u = u_1e_1 + u_2e_2 + u_3e_3 + u_4, \tag{34}$$

the transformation (26) gives for the components of x precisely equations (10) for the KS transformation. Moreover (32) gives

$$r\Omega(t) = 2(u_1\dot{u}_4 - u_4\dot{u}_1 - u_2\dot{u}_3 + u_3\dot{u}_2). \tag{35}$$

The constraint condition (15) (which plays such an important part in the KS transformation), when written with t as independent variable instead of s by using (11), is simply the condition that $\Omega(t)$ should vanish. Thus the KS transformation (10) together with the constraint condition (15) has a simple interpretation: the parameters u_α are the components of the quaternion which through the transformation (26) maps the unit vector along the Ox_1 axis into the position vector x of the moving particle, while the unit vectors along Ox_2 and Ox_3 are mapped into vectors which with x form an orthogonal triad having at each instant zero angular velocity about x.

5. The relation between Kepler motion and the harmonic oscillator

We obtain the equations which $u(t)$ must satisfy if $x(t)$ given by (26) satisfies the equation of motion (13) for a Kepler orbit. First note that

$$\dot{x} = 2\dot{\bar{u}}e_1 u + \chi = 2\bar{u}e_1\dot{u} - \chi, \tag{36}$$

where

$$\chi = \bar{u}e_1\dot{u} - \dot{\bar{u}}e_1u = r\Omega(t). \tag{37}$$

As we have seen, it is possible to choose $u(t)$ so that $\chi = 0$ for all t, but at this stage we leave this choice open. From (36) it follows that

$$|\dot{x}|^2 = 4|u|^2|\dot{u}|^2 - \chi^2 \tag{38}$$

and so the energy equation for the motion satisfying (13) may be written

$$E = \tfrac{1}{2}m|\dot{x}|^2 - \kappa^2|x|^{-1} = 2m|u|^2|\dot{u}|^2 - \tfrac{1}{2}m\chi^2 - \kappa^2|u|^{-2}. \tag{39}$$

The angular momentum $\boldsymbol{L}$ is given by

$$\boldsymbol{L} = m\boldsymbol{x} \times \dot{\boldsymbol{x}} = m|u|^2(\dot{\bar{u}}u - \bar{u}\dot{u}) - m\chi\bar{u}e_1u, \tag{40}$$

and the equation of motion (13) becomes

$$2(\mathrm{d}/\mathrm{d}t)(|u|^2\dot{u}) - u[2|\dot{u}|^2 - (\kappa^2/m)|u|^{-4}] + 2e_1\chi\dot{u} + e_1u\dot{\chi} = 0. \tag{41}$$

Now take $\chi = 0$, which as we have seen is equivalent to the constraint condition (15), and replace t as independent variable by s defined by (11). Equations (40) and (39) then simplify to give

$$m(\bar{u}'u - \bar{u}u') = \boldsymbol{L}, \tag{42}$$

$$\tfrac{1}{2}m|u'|^2 - \tfrac{1}{4}E|u|^2 = \tfrac{1}{4}\kappa^2. \tag{43}$$

The equation of motion (41), using (43), reduces to

$$u'' = (E/2m)u, \tag{44}$$

showing that the components of the quaternion u satisfy the equations of motion for a 4D harmonic oscillator in agreement with the result (14) obtained by Kustaanheimo and Stiefel (1965). This direct derivation of (44) using the quaternion formalism also has the advantage that it gives an expression for the angular momentum $\boldsymbol{L}$ of the Kepler orbit in terms of the variables in u space. From (42) it follows that the components of $\boldsymbol{L}$ along the fixed coordinate axes corresponding to the unit quaternions e_1, e_2 and e_3 are given in terms of the six constant components $U_{\alpha\beta}$ of the angular momentum of the 4D oscillator by

$$L_1 = 4U_{23} = -4U_{41}, \qquad L_2 = 2(U_{31} - U_{42}), \qquad L_3 = 2(U_{12} - U_{43}), \tag{45}$$

where

$$U_{\alpha\beta} = m(u_\alpha u'_\beta - u_\beta u'_\alpha), \qquad \alpha, \beta = 1, 2, 3, 4. \tag{46}$$

The constraint (15) requires

$$U_{23} + U_{41} = 0. \tag{47}$$

It is straightforward to show that the components of $\boldsymbol{L}$ referred to the moving axes corresponding to the unit quaternions f_2 and f_3 of (30) are given by

$$\begin{aligned} l_2 &= \boldsymbol{L}\cdot f_2 = m(\bar{u}e_2u' - \bar{u}'e_2u) = -2(U_{31} + U_{42}), \\ l_3 &= \boldsymbol{L}\cdot f_3 = m(\bar{u}e_3u' - \bar{u}'e_3u) = -2(U_{12} + U_{43}). \end{aligned} \tag{48}$$

Thus l_2 and l_3 are the two remaining constants of the motion arising from the six components of $U_{\alpha\beta}$.

Using (29), $u(t)$ may be expressed as

$$u = \bar{\zeta}_A - e_3\zeta_B, \tag{49}$$

where

$$\begin{aligned}\zeta_A &= r^{1/2}\cos\tfrac{1}{2}\theta\,\exp[e_1(\psi+\phi)/2] = u_4 - e_1u_1,\\ \zeta_B &= r^{1/2}\sin\tfrac{1}{2}\theta\,\exp[e_1(\psi-\phi)/2] = -u_3 - e_1u_2.\end{aligned} \tag{50}$$

Then (26) gives for the components of $\boldsymbol{x}$

$$x_1 = |\zeta_A|^2 - |\zeta_B|^2, \qquad x_2 + e_1x_3 = 2\zeta_A\bar{\zeta}_B. \tag{51}$$

With x_1, x_2, x_3 replaced by z, x and y respectively, these give the transformation used by Cornish (1984) to reduce the Schrödinger equation for the hydrogen atom to that for a 4D harmonic oscillator. In terms of ζ_A and ζ_B the constraint (15) becomes

$$\zeta_A\bar{\zeta}'_A - \bar{\zeta}_A\zeta'_A = -(\zeta_B\bar{\zeta}'_B - \bar{\zeta}_B\zeta'_B), \tag{52}$$

which express the constraint condition in terms of coupled oscillators in the ζ_A and ζ_B planes, their angular momenta being equal and opposite. The angular momentum $\boldsymbol{L}$ of the Kepler orbit in $\boldsymbol{x}$ space is given by

$$\boldsymbol{L} = 2m(\zeta'_A\bar{\zeta}_A - \zeta_A\bar{\zeta}'_A) + 2e_3m(\zeta'_B\bar{\zeta}_A - \bar{\zeta}'_A\zeta_B). \tag{53}$$

The transformation given in § 2 for the 2D case may be recovered in several ways. For example, $\zeta_A = \bar{\zeta}_B = 2^{-1/2}\zeta$ satisfies the constraint (52) and reduces the transformation (51) to (3) for orbits in the Ox_2x_3 plane. For orbits in the Ox_1x_2 plane a suitable choice for u in (26), which satisfies the constraint (15), is

$$u = v_1 - e_3v_2, \tag{54}$$

and the transformation (10) reduces to (4).

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