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Abstract

The Kustaanheimo–Stiefel (KS) transformation maps the non-linear and singular equations of motion of the three-dimensional Kepler problem to the linear and regular equations of a four-dimensional harmonic oscillator. It is used extensively in studies of the perturbed Kepler problem in celestial mechanics and atomic physics. In contrast to the conventional matrix-based approach, the formulation of the KS-transformation in the language of geometric Clifford algebra offers the advantages of a clearer geometrical interpretation and greater computational simplicity. It is demonstrated that the geometric algebra formalism can readily be used to derive a Lagrangian and Hamiltonian description of the KS dynamics in arbitrary static electromagnetic fields.

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1. Introduction

The Kepler problem belongs to the simplest systems of classical mechanics. A detailed understanding of its properties is of equally fundamental importance to celestial mechanics and to atomic physics. In both areas, it is of interest to describe, either by means of analytic approximations or numerical computation, the impact of additional non-Coulombic forces on the dynamics. In its original form, the equation of motion

$$\frac{\mathrm{d}^2 x}{\mathrm{d}t^2} = -\frac{x}{|x|^3} \tag{1}$$

is not well suited to this purpose because it is highly non-linear and exhibits a singularity at the Coulomb centre where the force diverges. For numerical studies of the dynamics, it is mandatory to find a representation of the equations of motion which avoids this singularity.

For the one-dimensional Kepler motion, it was already found by Euler [1] that the introduction of a square-root coordinate $u = \sqrt{x}$ and a fictitious time τ defined by $\mathrm{d}t = x\,\mathrm{d}\tau$ reduces the Kepler equation of motion (1) to the equation of motion of a one-dimensional harmonic oscillator

$$\frac{\mathrm{d}^2 u}{\mathrm{d}\tau^2} + 2Eu = 0 \tag{2}$$

where E is the energy of the Kepler motion. Equation (2) is not only void of singularities, it is also linear and thus forms a much more convenient basis for analytic calculations.

Generalizing this approach, Levi-Cività [2] regularized the two-dimensional Kepler problem by combining the two spatial coordinates into a complex number $x = x_1 + \mathrm{i}x_2$ and introducing a complex square-root coordinate $u = \sqrt{x}$, which together with the fictitious-time transformation $\mathrm{d}t = |x|\,\mathrm{d}\tau$ reduces the Kepler problem to a two-dimensional harmonic oscillator.

Attempts to extend this regularization scheme to the three-dimensional Kepler problem failed, until in 1964 Kustaanheimo and Stiefel [3, 4] proposed the introduction of four regularizing coordinates instead of three, and thereby achieved the reduction of the three-dimensional Kepler problem to a four-dimensional harmonic oscillator. This transformation, which is known as the Kustaanheimo–Stiefel (KS) transformation, is discussed in detail in the monograph by Stiefel and Scheifele [5]. Beyond its importance to celestial mechanics, it has proven to be an essential tool for investigating the complicated classical dynamics of the hydrogen atom in crossed electric and magnetic fields [6–8].

Customarily, the KS-transformation is expressed in the language of matrix algebra, which not only necessitates awkward computations of vector and matrix components, but also lacks a transparent geometric interpretation. An alternative formulation in terms of the geometric algebra of Euclidean three-space was introduced by Hestenes [9]. In this formalism, the four KS coordinates are interpreted as the components of a position spinor and are thus given a clear geometric meaning. In addition, the formalism offers computational advantages over the conventional matrix-based approach because it unites the four coordinates into a single spinor.

In this paper, I elaborate on the geometric algebra formulation of the KS-transformation. The calculations will amply demonstrate the advantages of the geometric algebra over the matrix-based formalism. The terminology used is adapted to applications in atomic physics. In particular, I discuss the motion of an electron of unit mass and negative unit charge under the influence of the nucleus and arbitrary static external electromagnetic fields. Nevertheless, the actual scope of the results is much broader. They apply equally to celestial mechanics or any other field of physics governed by the equations of motion of a perturbed Kepler problem.

A brief introduction into the properties of geometric algebra needed here is given in section 2, where the notation used in what follows is also explained. In section 3, the geometric algebra formulation of the KS-transformation is introduced and its relation to the matrix-based approach is established. The spinor equation of motion given by Hestenes [9] is derived. In section 4, a Lagrangian and Hamiltonian formulation of the KS spinor dynamics is derived. It cannot be obtained by a simple change of variables because the KS-transformation introduces a non-physical fourth degree of freedom and a pseudotime parameter. Nevertheless, it is demonstrated that the geometric algebra formulation readily lends itself to an incorporation into the Lagrangian and Hamiltonian formulations of dynamics. At the same time, the well-known KS Hamiltonian [6, 10, 11], which is restricted to homogeneous external electromagnetic fields, is generalized to arbitrary static fields. Section 5 presents the explicit solution of the spinor equation of motion in a pure Coulomb field and gives the constants of motion in terms of the KS spinor.

2. Introduction to geometric algebra

Geometric algebra is an algebraic system designed to represent the geometric properties of Euclidean space in the most comprehensive and systematic way possible. It was pioneered by Hermann Grassmann and William Kingdon Clifford during the nineteenth century. Beginning in the 1960s David Hestenes extended the algebraic techniques of Grassmann and Clifford by a differential and integral calculus within the geometric algebra, which he called geometric calculus [12].

   This section gives only a sketch of geometric algebra as far as it is needed in the present work. A thorough introduction to the geometric algebra of Euclidean three-space, with a detailed discussion of applications to classical mechanics, can be found in [9]. A detailed presentation of the mathematical properties of the geometric algebra is given in [12].

2.1. The geometric algebra of Euclidean three-space

The mathematical description of geometrical quantities customarily employs (real) scalars to represent non-directional quantities and vectors to represent directed line segments. The geometric algebra supplements these concepts with quantities representing directed area segments (bivectors) and oriented volume elements (trivectors). In addition, it introduces a multiplication of vectors called the geometric product that allows an area segment to be regarded as the product of two orthogonal vectors spanning the appropriate plane and a volume element as the product of three vectors spanning the space.

   Formally, the construction of the geometric product starts by picking a right-handed frame of orthonormal unit vectors σ_1, σ_2 and σ_3. For them, the geometric product is defined by the relation

$$\sigma_i \sigma_j + \sigma_j \sigma_i = 2\delta_{ij}. \tag{3}$$

The reader may note that the defining relation (3) is the same as obeyed by the Pauli spin matrices. It is important, however, to retain the interpretation of the σ_i as ordinary vectors instead of regarding them as matrices. In addition to (3), the geometric product is required to be associative and to obey the distributive law with respect to the usual addition of vectors. The latter property allows one to extend the definition of the geometric product to arbitrary vectors. For $a = \sum_{i=1}^{3} a_i \sigma_i$ and $b = \sum_{i=1}^{3} b_i \sigma_i$, one finds

$$ab = a_1 b_1 + a_2 b_2 + a_3 b_3 + (a_2 b_3 - a_3 b_2)\sigma_2 \sigma_3$$
$$+ (a_3 b_1 - a_1 b_3)\sigma_3 \sigma_1 + (a_1 b_2 - a_2 b_1)\sigma_1 \sigma_2. \tag{4}$$

The scalar terms of this equation comprise the scalar product $a \cdot b$. In addition, there are bivector terms containing the product of two orthogonal vectors. Following what was said above, they should be taken to represent the area spanned by a and b. This interpretation can be confirmed by noting that the coefficients of the bivector terms are the components of the vector cross product $a \times b$ that yields a vector orthogonal to the plane spanned by a and b. Indeed, with the help of the unit trivector

$$I = \sigma_1 \sigma_2 \sigma_3 \tag{5}$$

equation (4) can be rewritten as

$$ab = a \cdot b + I a \times b \tag{6}$$

which neatly unifies the scalar and vector products. As the scalar product is symmetric in its factors whereas the vector product is anti-symmetric, these products can be recovered from

the geometric product via

$$a \cdot b = \frac{1}{2}(ab + ba) \qquad a \times b = \frac{1}{2I}(ab - ba). \tag{7}$$

In particular, parallel vectors commute under the geometric product whereas perpendicular vectors anti-commute, and any vector a satisfies $aa = a \cdot a$.

Note that (6) contains a sum of quantities of different types, a scalar and a bivector. More generally, an arbitrary element of the geometric algebra, called a multivector, can be written as a sum of a scalar, a vector, a bivector and a trivector. The pure-grade parts of any multivector can be extracted by means of a grade projector. Let $\langle A \rangle_k$ be the grade-k part of the multivector A. Due to its particular importance, the scalar projector can be abbreviated as $\langle A \rangle = \langle A \rangle_0$, and the scalar product of two multivectors A and B is defined by

$$A * B = \langle AB \rangle. \tag{8}$$

For vectors, this agrees with the scalar dot product. Any two multivectors commute under the scalar product:

$$A * B = B * A. \tag{9}$$

In a term containing different kinds of products, the scalar product as well as the vector cross product are understood to take precedence over the geometric product. This convention has already been used in (6).

A multivector which contains only parts of even grades, i.e., scalars and bivectors, is referred to as an even multivector. The even multivectors form a subalgebra of the full geometric algebra.

Finally, the reversion $A^\dagger$ of a multivector A is obtained by interchanging the order of vectors in any geometric product. Thus, bivectors and trivectors change sign under reversion, whereas scalars and vectors remain unchanged. Formally, the reversion can be defined by the properties $a^\dagger = a$ for any vector a and

$$(AB)^\dagger = B^\dagger A^\dagger \qquad (A + B)^\dagger = A^\dagger + B^\dagger \tag{10}$$

for multivectors A and B.

2.2. Rotations in the geometric algebra

Within the geometric algebra, rotations are conveniently represented in the form

$$a \mapsto \mathrm{R}(a) = RaR^\dagger \tag{11}$$

with an even multivector R satisfying the normalization condition

$$RR^\dagger = 1. \tag{12}$$

Conversely, any normalized even multivector describes a rotation. An arbitrary even multivector satisfies $\alpha = UU^\dagger \geqslant 0$, so that $U = \sqrt{\alpha}R$ is a multiple of a rotor R. Therefore,

$$UaU^\dagger = \alpha RaR^\dagger \tag{13}$$

and U describes a rotation–dilatation of three-space. In particular,

$$UaU^\dagger = \langle UaU^\dagger \rangle_1 \tag{14}$$

is a vector for any even multivector U and any vector a.

A rotation can be characterized by specifying two vectors a and b so that a is mapped to b by a rotation in the plane $\langle ab \rangle_2$ spanned by a and b. The rotor R describing this rotation is

$$R = \frac{1 + ba}{|a + b|} = \frac{1 + ba}{\sqrt{2(1 + a \cdot b)}}. \tag{15}$$

If, alternatively, a rotation is characterized by its rotation axis, given by a unit vector n, and a rotation angle φ, the pertinent rotor reads

$$R = e^{-In\varphi/2} \tag{16}$$

where the exponential function of an arbitrary multivector is defined by the familiar power series

$$e^A = \sum_{n=0}^{\infty} \frac{A^n}{n!}. \tag{17}$$

It satisfies the 'power law' relation

$$e^{A+B} = e^A e^B \tag{18}$$

if $AB = BA$ and

$$e^A B = B e^A \qquad \text{if} \quad AB = BA \tag{19}$$

$$e^A B = B e^{-A} \qquad \text{if} \quad AB = -BA. \tag{20}$$

2.3. The multivector derivative

The formalism of the multivector derivative provides a differential calculus for arbitrary multivector functions. Let $F(X)$ be a smooth multivector-valued function of the multivector argument X. Neither the grades contained in X nor in F are specified. The directional derivative in the direction of a fixed multivector A is defined by

$$A * \partial_X F(X) = \left. \frac{\mathrm{d}F(X + \tau P_X(A))}{\mathrm{d}\tau} \right|_{\tau=0} \tag{21}$$

where $P_X(A)$ projects A onto the grades contained in X. (21) agrees with the familiar definition of the directional derivative.

Let $e_J, J = 1, \ldots, 8$ be a basis of the geometric algebra and e^J its dual basis, i.e., $e_J * e^K = \delta_J^K$. The multivector derivative is then defined to be

$$\partial_X = \sum_J e^J e_J * \partial_X. \tag{22}$$

It inherits the algebraic properties of its argument X. In particular, ∂_X contains the same grades as X. Note that the scalar product $A * \partial_X$ is indeed the directional derivative in the direction A, justifying the notation introduced in (21). For a vector argument x, the multivector derivative ∂_x reduces to the vector derivative, which is analogous to the familiar nabla operator.

Both the directional derivative and the multivector derivative are linear operators and satisfy Leibniz' rule

$$A * \partial_X (F(X)G(X)) = (A * \partial_X F(X))G(X) + F(X)(A * \partial_X G(X)) \tag{23}$$

$$\partial_X (F(X)G(X)) = \overset{*}{\partial}_X \overset{*}{F}(X)G(X) + \overset{*}{\partial}_X F(X) \overset{*}{G}(X). \tag{24}$$

In (24), the overstars indicate the functions to be differentiated. Note that the second term in (24) is in general different from $F(X)(\partial_X G(X))$, because due to its multivector properties the multivector derivative does not commute with F even if $F(X)$ is not differentiated. The directional derivative, in contrast, is a scalar differential operator that commutes with any

multivector that is not to be differentiated. For this reason, it is often convenient to write the multivector derivative as

$$\partial_X = \partial_A A * \partial_X. \tag{25}$$

This form decomposes ∂_X into a multivector ∂_A and a scalar differential operator $A * \partial_X$, which can be moved freely among multivectors.

In addition, the directional derivative satisfies the chain rule

$$A * \partial_X F(G(X)) = (A * \partial_X G(X)) * \partial_G F(G) \tag{26}$$

which is useful in many calculations.

A fundamental result concerning the multivector derivative is

$$\partial_X \langle XA \rangle = \partial_X \langle AX \rangle = P_X(A) \tag{27}$$

for any multivector A. As a consequence,

$$\partial_X \langle X^\dagger A \rangle = \partial_X \langle AX^\dagger \rangle = P_X(A^\dagger). \tag{28}$$

3. The spinor equation of motion

The KS-transformation in three dimensions can be found by representing an arbitrary position in space not by its position vector x, but by a position spinor, i.e., the rotation–dilatation operator transforming a fixed reference vector into the position vector x. As explained in 2, a rotation–dilatation of the reference vector σ_3 is represented in the geometric algebra by an even multivector U according to

$$x = \tfrac{1}{2} U \sigma_3 U^\dagger. \tag{29}$$

The factor $\tfrac{1}{2}$ was introduced here to stay in touch with earlier applications of the KS-transformation to atomic dynamics [10, 11], although the present formulation of the theory would suggest dropping it. It implies the normalization

$$U^\dagger U = U U^\dagger = 2r = 2|x|. \tag{30}$$

Up to normalization, the ansatz (29) reproduces the square-root coordinates introduced by Euler and Levi-Cività, respectively, if it is applied to spaces of one or two dimensions.

Given a position vector x, the choice of the spinor U is not unique. More precisely, the gauge transformation

$$U \mapsto U \, \mathrm{e}^{-I_3 \alpha/2} \tag{31}$$

with an arbitrary real parameter α does not alter x, because the additional exponential factor describes a rotation of the reference vector σ_3 around itself. In view of (29), (31) can also be written as

$$U \mapsto \frac{U}{\sqrt{2r}} \, \mathrm{e}^{-I_3 \alpha/2} \frac{U^\dagger}{\sqrt{2r}} U = \mathrm{e}^{-I x \alpha/2r} U. \tag{32}$$

In this form, the gauge transformation is interpreted as describing a rotation of the final vector x around itself that is performed after the mapping of σ_3 to x. Both of these alternative interpretations clarify why a position spinor representation in three dimensions must introduce a fourth degree of freedom. In lower dimensions, a rotation does not leave any vector invariant, so that the spinor transformation does not possess a gauge degree of freedom. It is also clear from (31) or (32) that all fibres of the KS-transformation except $U = 0$ are circles in spinor space.

The inverse KS-transformation can be found from equation (15) by adapting the normalization to (30). The position spinors corresponding to a vector $\boldsymbol{x}$ are given by

$$U = \frac{r + \boldsymbol{x}\boldsymbol{\sigma}_3}{\sqrt{r + z}} \, \mathrm{e}^{-I_3\alpha/2} \tag{33}$$

with arbitrary real α.

In components, the spinor U can be represented as $U = u_0 + I\boldsymbol{u}$ with $\boldsymbol{u} = \sum_{k=1}^{3} u_k \boldsymbol{\sigma}_k$. The transformation (29) then decomposes into

$$x = u_1 u_3 - u_0 u_2 \qquad y = u_1 u_0 + u_2 u_3 \qquad z = \tfrac{1}{2}\left(u_0^2 - u_1^2 - u_2^2 + u_3^2\right). \tag{34}$$

Up to renumbering the components, this agrees with the conventions of [10, 11].

To obtain an equation of motion for U, time derivatives of U must be calculated. Differentiating (29) leads to

$$\dot{\boldsymbol{x}} = \tfrac{1}{2}\dot{U}\boldsymbol{\sigma}_3 U^\dagger + \tfrac{1}{2}U\boldsymbol{\sigma}_3\dot{U}^\dagger = \langle \dot{U}\boldsymbol{\sigma}_3 U^\dagger \rangle_1. \tag{35}$$

Equation (35) obviously cannot be solved for $\dot{U}$ because the time derivative of the gauge parameter α in (31) cannot be determined from the dynamics of the position vector. To arrive at an equation of motion for U, I must therefore impose a constraint on α. To find a suitable way of doing so, note that the gauge transformation (31) with a time-dependent α leads to the substitution

$$\dot{U} \mapsto \dot{U}\,\mathrm{e}^{-I_3\alpha/2} - \frac{\dot{\alpha}}{2}U I_3\,\mathrm{e}^{-I_3\alpha/2} \tag{36}$$

and thus

$$\dot{U}\boldsymbol{\sigma}_3 U^\dagger \mapsto \dot{U}\boldsymbol{\sigma}_3 U^\dagger - \dot{\alpha}r I. \tag{37}$$

Therefore, a time-dependent gauge transformation introduces a pure trivector contribution into the product $\dot{U}\boldsymbol{\sigma}_3 U^\dagger$. It can be used to eliminate the trivector component altogether, i.e. to require

$$\langle \dot{U}\boldsymbol{\sigma}_3 U^\dagger \rangle_3 = 0 \tag{38}$$

which means that $\dot{U}$ is chosen such as not to contain a component of motion in the direction of the gauge degree of freedom. In view of the interpretation of the gauge transformation associated with (32), this means that there is no rotation around the instantaneous position vector $\boldsymbol{x}$. If the constraint (38) is adopted, (35) can be solved for $\dot{\boldsymbol{x}}$ to yield

$$\dot{\boldsymbol{x}} = \dot{U}\boldsymbol{\sigma}_3 U^\dagger \tag{39}$$

and

$$\dot{U} = \dot{\boldsymbol{x}}U^{\dagger-1}\boldsymbol{\sigma}_3 = \dot{\boldsymbol{x}}\frac{U}{2r}\boldsymbol{\sigma}_3. \tag{40}$$

As in the one- and two-dimensional cases, the regularization of the three-dimensional Kepler motion requires the introduction of a fictitious-time parameter τ. It is defined by

$$\mathrm{d}t = 2r\,\mathrm{d}\tau. \tag{41}$$

Derivatives with respect to τ will be denoted with a prime. Equation (40) then yields

$$U' = 2r\dot{U} = \dot{\boldsymbol{x}}U\boldsymbol{\sigma}_3. \tag{42}$$

A specific trajectory is characterized by initial conditions $\boldsymbol{x}$ and $\dot{\boldsymbol{x}}$. With the help of equations (33) and (42), they can be converted into initial conditions for the KS spinor U, unless $\boldsymbol{x} = 0$. In the latter case, which is of particular significance in atomic physics [10, 11, 13–16], $U = 0$, and the real-time velocity $\dot{\boldsymbol{x}}$ is infinite because the electron is located

in the Coulomb singularity. A suitable limiting process must then be applied to equation (42) to obtain a well-defined initial KS velocity U'. Details of this procedure can be found in [15].

For the second derivative of U, I obtain

$$
\begin{aligned}
U'' &= \left(\frac{\mathrm{d}}{\mathrm{d}\tau}\dot{x}\right)U\sigma_3 + \dot{x}U'\sigma_3 \\
&= 2r\ddot{x}U\sigma_3\frac{U^\dagger}{2r}U + \dot{x}^2 U \\
&= 2\left(\ddot{x}x + \frac{1}{2}\dot{x}^2\right)U.
\end{aligned}
\tag{43}
$$

Together with Newton's equation of motion

$$
\ddot{x} = -\frac{x}{r^3} + f
\tag{44}
$$

with an arbitrary non-Coulombic force f, equation (43) yields the spinor equation of motion in the form first given by Hestenes [9]:

$$
U'' = 2(E_{\mathrm{K}} + fx)U
\tag{45}
$$

where the Kepler energy

$$
E_{\mathrm{K}} = \frac{1}{2}\dot{x}^2 - \frac{1}{r}
\tag{46}
$$

denotes the sum of the kinetic and Coulombic potential energies.

In the special case of pure Kepler motion, i.e. $f = 0$, the Kepler energy E_{K} is equal to the total energy E and is conserved. In this case, (45) reduces to the linear equation of motion

$$
U'' = 2EU.
\tag{47}
$$

If $E < 0$, this is the equation of motion of a four-dimensional isotropic harmonic oscillator with frequency $\omega = \sqrt{-2E}$ with respect to τ.

If additional forces f are present, the Kepler energy is not conserved in general, so that the work done by the external forces must be taken into account [4]. This can easily be achieved if the external forces are generated by static electromagnetic fields, because the work done by a magnetic field B is zero, whereas an electric field $F = -\nabla V$ can be derived from a potential $V(x)$. In this case, the total energy $E = E_{\mathrm{K}} - V$ is conserved, so that the equation of motion reads

$$
U'' = 2(E + V(x) + fx)U
\tag{48}
$$

with $f = -F - \dot{x} \times B$. (The electron is assumed to carry negative unit charge.)

It finally remains to verify that the equation of motion (45) is consistent with the constraint (38). To prove this, first note that

$$
\xi = \langle U'\sigma_3 U^\dagger\rangle_3
\tag{49}
$$

is a constant of motion for any external forces f [4], because by (45)

$$
\begin{aligned}
\frac{\mathrm{d}\xi}{\mathrm{d}\tau} &= \langle U''\sigma_3 U^\dagger\rangle_3 + \underbrace{\langle U'\sigma_3 U'^\dagger\rangle_3}_{=0\,\mathrm{by}\,(14)} \\
&= \langle (E_{\mathrm{K}} + fx)\,x\rangle_3 \\
&= \langle E_{\mathrm{K}}x + r^2 f\rangle_3 \\
&= 0.
\end{aligned}
\tag{50}
$$

Therefore, if the initial conditions are chosen so that $\xi = 0$ at $\tau = 0$, equation (50) guarantees $\langle \dot{U}\sigma_3 U^\dagger\rangle_3 = 2r\xi = 0$ at all times.

4. Canonical formalism

In classical investigations of atoms in external fields, the Hamiltonian nature of the dynamics plays a central role. It is therefore essential to show how the spinor equation of motion found in the previous section can be derived in the context of a Lagrangian or Hamiltonian formalism. In the matrix theory of the KS-transformation, a Hamiltonian formulation is well known and widely applied in the literature [10, 11]. Due to the introduction of an additional degree of freedom and a fictitious-time parameter, it cannot be found by a straightforward change of variables. In this section, it will be shown that the application of geometric algebra allows an easy and general derivation of the Hamiltonian. At the same time, the Hamiltonian formalism will be generalized to arbitrary inhomogeneous static external fields.

4.1. Fictitious-time transformations

Elementary expositions of Lagrangian and Hamiltonian dynamics usually treat the time t as the externally prescribed independent variable fundamentally different from the spatial coordinates, velocities and momenta. The formalisms are then shown to be invariant under point transformations or canonical transformations, respectively, which may be time-dependent, but must not transform the time variable. However, both the Lagrangian and the Hamiltonian formalisms can be reformulated in such a way that it is possible to introduce an arbitrary orbital parameter τ and to treat the physical time t as an additional coordinate on the same footing as the spatial coordinates. This formalism is discussed in its full generality by Dirac [17, 18]. For the special case of autonomous Lagrangian dynamics and the simple form of the fictitious-time transformation used above, the full flexibility of Dirac's homogeneous formalism is not needed. Instead, the modifications needed to achieve the fictitious-time transformation can be derived in a straightforward manner from Hamilton's variational principle.

The Lagrangian equations of motion can be derived from the action functional

$$S = \int_{t_1}^{t_2} dt \, L(q(t), \dot{q}(t)) \tag{51}$$

by requiring that for the classical paths the variation of S with respect to the path $q(t)$ vanishes if the variation is performed with the initial and final times t_1 and t_2 and the coordinates $q(t_1)$ and $q(t_2)$ kept fixed. If a fictitious-time parameter τ is introduced by the prescription

$$dt = f(q, \dot{q}) \, d\tau \tag{52}$$

with an arbitrary function f, it is tempting to rewrite the action functional as

$$S = \int_{\tau_1}^{\tau_2} d\tau \, f(q, \dot{q}) L(q, \dot{q}) \tag{53}$$

and regard

$$\tilde{L} = f(q, \dot{q}) L(q, \dot{q}) = \frac{dt}{d\tau} L \tag{54}$$

as the Lagrangian describing the dynamics with respect to τ. However, this simple procedure is incorrect in general, because to derive the Lagrangian equations with respect to $\tilde{L}$ from (53), the variation of S has to be performed with the initial and final fictitious times τ_1 and τ_2 kept fixed, and due to (52) a variation of the path will alter the relation between t and τ, so that the initial and final physical times t_1 and t_2 will vary.

To establish the true relation between (51) and (53), I calculate the variation of (53) taking the variation of t into account, i.e. q and t are varied according to

$$q(\tau) \mapsto q(\tau) + \delta q(\tau) \qquad t(\tau) \mapsto t(\tau) + \delta t(\tau) \tag{55}$$

subject to the boundary conditions

$$\delta q(\tau_1) = \delta q(\tau_2) = 0 \tag{56}$$

and with τ_1 and τ_2 kept fixed. Under this variation,

$$
\begin{aligned}
\frac{d\tau}{dt} \mapsto \frac{d\tau}{d(t + \delta t)} &= \frac{1}{\frac{dt}{d\tau} + \frac{d\delta t}{d\tau}} \\
&= \frac{d\tau}{dt}\left(1 - \frac{d\tau}{dt}\frac{d\delta t}{d\tau}\right)
\end{aligned}
\tag{57}
$$

so that

$$\delta\frac{d\tau}{dt} = -\left(\frac{d\tau}{dt}\right)^2 \frac{d\delta t}{d\tau} \tag{58}$$

and hence

$$
\begin{aligned}
\delta\dot{q} &= \delta\left(\frac{dq}{d\tau}\frac{d\tau}{dt}\right) \\
&= \delta\left(\frac{dq}{d\tau}\right)\frac{d\tau}{dt} + \frac{dq}{d\tau}\delta\left(\frac{d\tau}{dt}\right) \\
&= \frac{d\delta q}{dt} - \dot{q}\frac{d\tau}{dt}\frac{d\delta t}{d\tau}.
\end{aligned}
\tag{59}
$$

The variation of (53) then reads

$$
\begin{aligned}
\delta S &= \int d\tau\left[\delta\left(\frac{dt}{d\tau}\right)L + \frac{dt}{d\tau}\left(\frac{\partial L}{\partial q}\delta q + \frac{\partial L}{\partial \dot{q}}\delta\dot{q}\right)\right] \\
&= \int d\tau\frac{d\delta t}{d\tau}\left(L - \dot{q}\frac{\partial L}{\partial \dot{q}}\right) + \int dt\left(\frac{\partial L}{\partial q}\delta q + \frac{\partial L}{\partial \dot{q}}\frac{d\delta q}{dt}\right) \\
&= -\int d\tau\frac{d\delta t}{d\tau}H + \int dt\left(\frac{\partial L}{\partial q} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}}\right)\delta q
\end{aligned}
\tag{60}
$$

where the customary partial integration was performed, the boundary conditions (56) were used and the Hamiltonian

$$H = \dot{q}\frac{\partial L}{\partial \dot{q}} - L \tag{61}$$

was introduced.

If only the second integral in the last line of (60) were present, it would yield the correct equations of motion. Thus, the action functionals (51) and (53) are equivalent if the Hamiltonian H vanishes. For autonomous systems, H is a constant of motion equal to the energy E. If the Lagrangian L is replaced with $L + E$, with E regarded as a constant, the equations of motion derived from L are unchanged, but the Hamiltonian (61) changes to $H - E = 0$. Thus, the dynamics of trajectories with energy E with respect to the fictitious-time parameter τ is described by the Lagrangian

$$\mathcal{L} = \frac{dt}{d\tau}(L + E) = f(q, \dot{q})(L + E). \tag{62}$$

This Lagrangian has to be written as a function of the coordinates q and the fictitious-time velocities q'. If the function f is independent of the velocities, the canonical momenta are invariant under the fictitious-time transformation, because $q' = f(q)\dot{q}$ and

$$\frac{\partial \mathcal{L}}{\partial q'} = f(q)\frac{\mathrm{d}\dot{q}}{\mathrm{d}q'}\frac{\partial L}{\partial \dot{q}} = \frac{\partial L}{\partial \dot{q}}. \tag{63}$$

From the time-transformed Lagrangian (62), the transformed Hamiltonian

$$\mathcal{H} = q'\frac{\partial \mathcal{L}}{\partial q'} - \mathcal{L} = f(q, \dot{q})(H - E) \tag{64}$$

is obtained by the usual Legendre transformation. It must be written as a function of the coordinates and momenta. In some cases, the passage from the Lagrangian to the Hamiltonian description of the dynamics is impossible because the relation $p = \partial\mathcal{L}(q, q')/\partial q'$ cannot be solved for q'. In these cases, the Hamiltonian (64) can be shown to describe the fictitious-time dynamics by a discussion of the modified Hamilton's principle analogous to the derivation of the Lagrangian $\mathcal{L}$ above.

4.2. Lagrangian description

The dynamics of an atomic electron under the combined influences of the nuclear Coulomb potential, an additional scalar potential $V(\boldsymbol{x})$ and a magnetic field represented by a vector potential $\boldsymbol{A}(\boldsymbol{x})$ is described by the Lagrangian

$$L = \frac{\dot{\boldsymbol{x}}^2}{2} + \frac{1}{r} + V(\boldsymbol{x}) - \boldsymbol{A} \cdot \dot{\boldsymbol{x}}. \tag{65}$$

This Lagrangian must be transformed to a Lagrangian $\mathcal{L}$ describing the fictitious-time dynamics of the position spinor U. With $f(q) = 2r = U^\dagger U$ by (41), the fictitious-time Lagrangian (62) reads

$$\mathcal{L} = \frac{1}{4}U'^\dagger U' + \frac{1}{8r}\langle (U'\boldsymbol{\sigma}_3 U^\dagger)^2 \rangle + EU^\dagger U + U^\dagger U V(\boldsymbol{x}) - \langle \boldsymbol{A}(\boldsymbol{x})U'\boldsymbol{\sigma}_3 U^\dagger \rangle + 2 \tag{66}$$

with $\boldsymbol{x} = \frac{1}{2}U\boldsymbol{\sigma}_3 U^\dagger$. If the constraint (38) is used, $\mathcal{L}$ simplifies to

$$\mathcal{L} = \tfrac{1}{2}U'^\dagger U' + EU^\dagger U + U^\dagger U V(\boldsymbol{x}) - \langle \boldsymbol{A}(\boldsymbol{x})U'\boldsymbol{\sigma}_3 U^\dagger \rangle + 2. \tag{67}$$

Both forms of the Lagrangian yield the same 'on-shell' dynamics for trajectories satisfying (38). Note that only the kinetic term is influenced by the constraint, whereas the potential and vector potential terms are not.

The momentum conjugate to U is given by

$$P = \partial_{U'}\mathcal{L} = \frac{1}{2r}\boldsymbol{\sigma}_3 U^\dagger \langle U'\boldsymbol{\sigma}_3 U^\dagger \rangle_1 - \boldsymbol{\sigma}_3 U^\dagger \boldsymbol{A} \tag{68}$$

which simplifies to

$$P = U'^\dagger - \boldsymbol{\sigma}_3 U^\dagger \boldsymbol{A} \tag{69}$$

if (38) is applied.

As the spinor equation of motion (45) is valid under the constraint (38) only, the Lagrangian $\mathcal{L}$ provides a suitable description of the dynamics if it reproduces (45) for trajectories satisfying (38). The simplified Lagrangian (67) can therefore be used. When equations of motion are derived from (67), the constraint (38) must be taken into account by a Lagrangian multiplier. I will now show, however, that the unconstrained equation of motion [19]

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\partial_{U'}\mathcal{L} - \partial_U \mathcal{L} = 0 \tag{70}$$

derived from (67) reproduces (45) without the constraint being explicitly dealt with, i.e. the Lagrangian multiplier to be introduced turns out to vanish identically. I therefore ignore it from the outset.

For the case of vanishing external potentials, (70) can easily be seen to yield

$$U''^{\dagger} - 2EU^{\dagger} = 0 \tag{71}$$

which is the reversion of (47). For the terms containing the potentials, the calculation of (70) is still straightforward, but requires a more intimate familiarity with the properties of the multivector derivative. I will therefore present the calculation in detail.

The contribution of the scalar potential term

$$\mathcal{V} = U^{\dagger} U V(\boldsymbol{x}(U)) \tag{72}$$

with $\boldsymbol{x}(U) = \frac{1}{2} U \boldsymbol{\sigma}_3 U^{\dagger}$ reads, by (24),

$$\partial_U \mathcal{V} = 2U^{\dagger} V(\boldsymbol{x}) + U^{\dagger} U \partial_U V(\boldsymbol{x}(U)). \tag{73}$$

The chain rule (26) then yields for any even multivector M

$$M * \partial_U V(\boldsymbol{x}(U)) = (M * \partial_U \boldsymbol{x}(U)) * \partial_{\boldsymbol{x}} V \tag{74}$$

with

$$\begin{aligned} M * \partial_U \boldsymbol{x}(U) &= (M * \partial_U) \tfrac{1}{2} U \boldsymbol{\sigma}_3 U^{\dagger} \\ &= \tfrac{1}{2} M \boldsymbol{\sigma}_3 U^{\dagger} + \tfrac{1}{2} U \boldsymbol{\sigma}_3 M^{\dagger} \\ &= \langle M \boldsymbol{\sigma}_3 U^{\dagger} \rangle_1. \end{aligned} \tag{75}$$

In the absence of a magnetic field the external force is $\boldsymbol{f} = \partial_{\boldsymbol{x}} V$, so that

$$M * \partial_U V(\boldsymbol{x}(U)) = \langle \langle M \boldsymbol{\sigma}_3 U^{\dagger} \rangle_1 \boldsymbol{f} \rangle = \langle M \boldsymbol{\sigma}_3 U^{\dagger} \boldsymbol{f} \rangle. \tag{76}$$

Thus,

$$\partial_U V = \partial_M (M * \partial_U V) = \boldsymbol{\sigma}_3 U^{\dagger} \boldsymbol{f} \tag{77}$$

and finally

$$\partial_U \mathcal{V} = 2U^{\dagger} V(\boldsymbol{x}) + 2U^{\dagger} \boldsymbol{x} \boldsymbol{f}. \tag{78}$$

This is the reversion of the scalar-potential terms in (45). Therefore, (78) together with (71) indeed yields the correct equation of motion.

To evaluate the contribution of the vector potential term

$$\mathcal{A} = \langle \boldsymbol{A}(\boldsymbol{x}) U' \boldsymbol{\sigma}_3 U^{\dagger} \rangle \tag{79}$$

to (70), first note that

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}\tau} \partial_{U'} \mathcal{A} &= \frac{\mathrm{d}}{\mathrm{d}\tau} (\boldsymbol{\sigma}_3 U^{\dagger} \boldsymbol{A}(\boldsymbol{x})) \\ &= \boldsymbol{\sigma}_3 U'^{\dagger} \boldsymbol{A}(\boldsymbol{x}) + \boldsymbol{\sigma}_3 U^{\dagger} (\boldsymbol{x}' \cdot \partial_{\boldsymbol{x}}) \boldsymbol{A}(\boldsymbol{x}). \end{aligned} \tag{80}$$

By Leibniz' rule and (35),

$$\begin{aligned} \partial_U \mathcal{A} &= \overset{*}{\partial}_U \langle \boldsymbol{A} U' \boldsymbol{\sigma}_3 \overset{*}{U}^{\dagger} \rangle + \overset{*}{\partial}_U \langle \overset{*}{\boldsymbol{A}} U' \boldsymbol{\sigma}_3 U^{\dagger} \rangle \\ &= \boldsymbol{\sigma}_3 U'^{\dagger} \boldsymbol{A} + \partial_U \langle \boldsymbol{A}(\boldsymbol{x}(U)) \boldsymbol{x}' \rangle. \end{aligned} \tag{81}$$

The second term on the right-hand side can be evaluated by first calculating directional derivatives. For an arbitrary even M, (75) and the chain rule (26) yield

$$
\begin{aligned}
(M * \partial_U)\langle A(x(U))x'\rangle &= (M * \partial_U A) * \partial_A \langle Ax'\rangle \\
&= \langle (M * \partial_U A(x(U)))x'\rangle \\
&= \langle (M * \partial_U x) * \partial_x A x'\rangle \\
&= \langle \langle \langle M\sigma_3 U^\dagger\rangle_1 \partial_x\rangle A x'\rangle \\
&= \langle M\sigma_3 U^\dagger \partial_x\rangle \langle A x'\rangle
\end{aligned}
\tag{82}
$$

so that

$$
\begin{aligned}
\partial_U \langle A(x(U))x'\rangle &= \partial_M (M * \partial_U)\langle A(x(U))x'\rangle \\
&= \sigma_3 U^\dagger \partial_x (A \cdot x').
\end{aligned}
\tag{83}
$$

Equations (80), (81) and (83) combine to

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}\tau}\partial_{U'}\mathcal{A} - \partial_U \mathcal{A} &= \sigma_3 U^\dagger((x' \cdot \partial_x)A - \partial_x(A \cdot x')) \\
&= -\sigma_3 U^\dagger(x' \times (\partial_x \times A)) \\
&= -2U^\dagger x(\dot{x} \times B)
\end{aligned}
\tag{84}
$$

which is the reversion of the magnetic-field contribution to (45).

Note that the derivation given here is valid for arbitrary external potentials V and A, whereas conventional treatments restrict themselves to the special case of homogeneous external fields. It can obviously be further generalized to include conservative forces of non-electromagnetic origin. Also note that the geometric algebra formalism allows one to do the calculations in a straightforward manner without having to resort to component decompositions of any of the vectorial or spinorial quantities involved.

4.3. Hamiltonian description

The transition from a Lagrangian to a Hamiltonian description of the dynamics leads from the Lagrangian (66) or (67), depending on whether or not the constraint (38) is applied, to the Hamiltonian

$$
\mathcal{H} = (U' * \partial_{U'})\mathcal{L} - \mathcal{L}
\tag{85}
$$

in which the velocity U' has to be expressed in terms of the momentum P. The transformation requires that the relation (68) or (69) between velocity and momentum can be solved for the velocity, which is impossible in the case of (68). Thus, the constraint (38) is not only needed to obtain an unambiguous equation of motion for U, but also serves as a condition for a Hamiltonian description of the spinor dynamics to exist. If it is imposed and an inessential constant of 2 is added, the Hamiltonian reads

$$
\mathcal{H} = \tfrac{1}{2}(P^\dagger + AU\sigma_3)(P + \sigma_3 U^\dagger A) - EU^\dagger U - U^\dagger U V(x) = 2.
\tag{86}
$$

Because it is time-independent, the Hamiltonian (86) is a constant of motion. To describe the physical dynamics, its value must be chosen to be 2, whereas the physical energy E appears as a parameter in $\mathcal{H}$.

The equations of motion derived from (86) read

$$
\begin{aligned}
U' &= \partial_P \mathcal{H} = P^\dagger + AU\sigma_3 \\
P' &= -\partial_U \mathcal{H} \\
&= -2EU^\dagger - 2U^\dagger V(x) - 2U^\dagger x \partial_x V \\
&\quad - \sigma_3(P + \sigma_3 U^\dagger A)A - \sigma_3 U^\dagger \overset{*}{\partial}_x \langle \overset{*}{A} x'\rangle
\end{aligned}
\tag{87}
$$

where
$$x' = U\sigma_3 U'^\dagger = U\sigma_3 P + U^\dagger U A \tag{88}$$
was used. In terms of coordinates and momenta, the constraint (38) reads
$$\langle U\sigma_3 P\rangle_3 = 0. \tag{89}$$
Equation (89) is equivalent to (38) both in the presence and in the absence of a magnetic field. Taken together, (87) and (88) lead back to the equation of motion (45).

Finally, let me mention an important subtlety regarding the component decomposition of the spinor equation. If, according to (34), U is represented as $U = u_0 + I\boldsymbol{u}$ with $\boldsymbol{u} = \sum_{k=1}^3 u_k\sigma_k$ and p_k denotes the momentum component conjugate to u_k, the spinor momentum is $P = p_0 - I\boldsymbol{p}$ with $\boldsymbol{p} = \sum_{k=1}^3 p_k\sigma_k$. The negative sign is necessary because in the spinor formulation the bivector $I_k p_k$ is conjugate to $I_k u_k$. Dropping the bivector factors I_k leads to the stated result.

5. The Kepler problem

The unperturbed Kepler motion is described by the Hamiltonian
$$\mathcal{H} = \tfrac{1}{2}P^\dagger P - EU^\dagger U = 2. \tag{90}$$
The equations of motion derived from (90) are
$$U' = P^\dagger \qquad P' = 2EU^\dagger \tag{91}$$
or, as in (47),
$$U'' = 2EU.$$
If $E < 0$, this is the equation of motion of an isotropic four-dimensional harmonic oscillator, whose general solution reads
$$U = A\cos(\sqrt{-2E}\,\tau) + B\sin(\sqrt{-2E}\,\tau) \tag{92}$$
with two constant even multivectors A and B bound, by (38) and (90), to satisfy
$$\langle A\sigma_3 B^\dagger\rangle_3 = 0 \tag{93}$$
and
$$A^\dagger A + B^\dagger B = -\frac{2}{E}. \tag{94}$$

In the case of the pure Kepler motion, the angular momentum vector $\boldsymbol{L}$ and the Lenz vector $\boldsymbol{\epsilon}$ are conserved. Together, they uniquely specify an orbit [9]. I will now derive the KS-transformed expressions for these constants of motion. Throughout, the validity of the constraint (38) will be assumed.

The angular momentum vector is given by
$$\boldsymbol{L} = \boldsymbol{x} \times \dot{\boldsymbol{x}} = -I\langle\boldsymbol{x}\dot{\boldsymbol{x}}\rangle_2. \tag{95}$$
Within the geometric algebra, it is more convenient to introduce the angular momentum bivector
$$l = I\boldsymbol{L} = \langle\boldsymbol{x}\dot{\boldsymbol{x}}\rangle_2 \tag{96}$$
which specifies the orbital plane instead of the direction perpendicular to it. By (29), (35) and (38),
$$\begin{aligned} l &= \langle\tfrac{1}{2}U\sigma_3 U^\dagger U\sigma_3\dot{U}^\dagger\rangle_2 \\ &= \tfrac{1}{2}\langle UU'^\dagger\rangle_2 \\ &= \tfrac{1}{2}\langle UP\rangle_2. \end{aligned} \tag{97}$$

That l is conserved can be verified by a straightforward differentiation. Alternatively, it can be checked that the Poisson bracket vanishes,

$$
\begin{aligned}
\{l, \mathcal{H}\} &= (\partial_P \mathcal{H}) * \partial_U l - (\partial_U \mathcal{H}) * \partial_P l \\
&= P^\dagger * \partial_U l + 2EU^\dagger * \partial_P l \\
&= \tfrac{1}{2}\langle P^\dagger P \rangle_2 + E \langle U^\dagger U \rangle_2 \\
&= 0.
\end{aligned}
\tag{98}
$$

Note how the Poisson bracket formalism extends not only to multivector coordinates U and P, but also to non-scalar arguments.

The Lenz vector is given by

$$
\begin{aligned}
\epsilon &= l\dot{x} - \frac{x}{r} \\
&= lP^\dagger \sigma_3 U^{-1} - U\sigma_3 U^{-1}.
\end{aligned}
\tag{99}
$$

To calculate the Poisson bracket $\{\epsilon, \mathcal{H}\}$, use $\{l, \mathcal{H}\} = 0$ and

$$
P^\dagger * \partial_U U^{-1} = -U^{-1} P^\dagger U^{-1}
\tag{100}
$$

to find

$$
\begin{aligned}
\{\epsilon, \mathcal{H}\} &= l\{P^\dagger \sigma_3 U^{-1}, \mathcal{H}\} - \{U\sigma_3 U^{-1}, \mathcal{H}\} \\
&= l(P^\dagger * \partial_U (P^\dagger \sigma_3 U^{-1}) + 2EU^\dagger * \partial_P (P^\dagger \sigma_3 U^{-1})) \\
&\quad - P^\dagger * \partial_U (U\sigma_3 U^{-1}) \\
&= l(-P^\dagger \sigma_3 U^{-1} P^\dagger U^{-1} + 2EU\sigma_3 U^{-1}) \\
&\quad - P^\dagger \sigma_3 U^{-1} + U\sigma_3 U^{-1} P^\dagger U^{-1} \\
&= [l(-P^\dagger \sigma_3 U^{-1} P^\dagger \sigma_3 U^\dagger + 2EUU^\dagger) \\
&\quad - P^\dagger U^\dagger + U\sigma_3 U^{-1} P^\dagger \sigma_3 U^\dagger]U^{\dagger^{-1}} \sigma_3 U^{-1}.
\end{aligned}
\tag{101}
$$

Due to the constraint (89),

$$
P^\dagger \sigma_3 U^\dagger = U\sigma_3 P
\tag{102}
$$

so that equation (101) simplifies to

$$
\begin{aligned}
\{\epsilon, \mathcal{H}\} &= [l(-P^\dagger P + 2EU^\dagger U) - P^\dagger U^\dagger + UP]U^{\dagger^{-1}} \sigma_3 U^{-1} \\
&= [-2l\mathcal{H} + 2\langle UP \rangle_2]U^{\dagger^{-1}} \sigma_3 U^{-1} \\
&= 0.
\end{aligned}
\tag{103}
$$

Thus, the Lenz vector ϵ is actually conserved.

6. Conclusion

The geometric algebra formulation of the KS-transformation endows the four KS coordinates with a clear geometric interpretation. It was shown in this paper that it also allows for an easy incorporation into a Lagrangian and Hamiltonian formulation of the KS theory. At the same time, the known KS Hamiltonian, that was restricted to homogeneous external fields, was generalized to describe the KS motion in arbitrary static external electromagnetic fields. This result is of interest beyond the realm of atomic physics because it is equally applicable to an arbitrary conservative non-electromagnetic force.

The calculations carried out here amply illustrate the power of the geometric algebra formulation of the KS theory. It can thus be expected to form a convenient starting point for analytic calculations in classical perturbation theory.

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