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Kustaanheimo–Stiefel Transformation of the Monopolar Hydrogen Atom into the Four-Dimensional Oscillator

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We show that the monopolar hydrogen atom is connected to a four-dimensional harmonic oscillator with a monopole-dependent constraint by the Kustaanheimo–Stiefel transformation.

1. INTRODUCTION AND THE EXTENDED HYDROGEN ATOM

The simplest atom, hydrogen, serves as a prototype for descriptions of more complicated many-electron atoms. It is given in textbooks as one of the few solvable problems in both classical and quantum physics. Almost all treatises on quantum mechanics and atomic physics treat selected aspects of the hydrogen atom. Yet despite this voluminous literature, research continues to reveal novel aspects of this elementary system. An example is the connection between the three-dimensional hydrogen atom and the four-dimensional isotropic harmonic oscillator by the Kustaanheimo–Stiefel (KS) transformation, which has been a subject of considerable interest in the last three decades [1–14]. Recently, we found an extended $U(1)$ monopole-dependent hydrogen atom [15] (it is a little different from the McIntosh–Cisneros–Zwanziger system, a charged spinless particle in a combined monopole plus scalar potential field [16,17]), whose Schrödinger equation reads

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$$H\psi = E\psi, \qquad H = \frac{\vec{\pi}^2}{2\mu} + \frac{1}{2\mu}\frac{q^2}{r^2} - \frac{\kappa}{r} \tag{1}$$

where μ is the reduced mass of the hydrogen atom, $\kappa = e^2$, $\vec{\pi} = \mathbf{p} - e\mathbf{A}$, $\mathbf{A}$ is the vector potential defined in two different regions R_a $(0 \le \theta \le \pi/2 + \delta)$ and R_b $(\pi/2 - \delta \le \theta \le \pi)$ as [18]

$$(A_r)_a = (A_\theta)_a = 0, \qquad (A_\phi)_a = \frac{g}{r\sin\theta}(1 - \cos\theta) = \frac{g}{r}\tan\frac{\theta}{2}$$

$$(A_r)_b = (A_\theta)_b = 0, \qquad (A_\phi)_b = -\frac{g}{r\sin\theta}(1 + \cos\theta) = -\frac{g}{r}\cot\frac{\theta}{2} \tag{2}$$

and $q = eg = 1/2 \times$ integer is the Dirac $U(1)$ magnetic monopole [19]. Parallel to the usual hydrogen atom, in the extended physical system there exist two conserved vectors

$$\mathbf{L} = \mathbf{r} \times \vec{\pi} - q\frac{\mathbf{r}}{r}, \qquad \mathbf{R} = \frac{1}{2\mu\kappa}(\vec{\pi} \times \mathbf{L} - \mathbf{L} \times \vec{\pi}) - \frac{\mathbf{r}}{\mathrm{r}} \tag{3}$$

which are the extended monopole-dependent angular momentum vector and the extended Laplace–Runge–Lenz–Pauli (LRLP) vector, respectively. Due to

$$\vec{\pi} \times \vec{\pi} = e\,\nabla \times \mathbf{A} = q\frac{\mathbf{r}}{r^3} \qquad \text{or} \tag{4}$$

$$[\pi_\alpha, \pi_\beta] = i\epsilon_{\alpha\beta\gamma} q \frac{x_\gamma}{r^3} \quad (\alpha, \beta, \gamma = 1, 2, 3)$$

one can easily verify that $\mathbf{L} = (L_1, L_2, L_3)$ and $\mathbf{B} = \sqrt{(-\mu\kappa^2/2E)}\,\mathbf{R} = (B_1, B_2, B_3)$ span the $SO(4)$ dynamic symmetry group, and the two corresponding extended monopole-dependent Pauli relations [20] are

$$\mathbf{L} \cdot \mathbf{B} = \mathbf{B} \cdot \mathbf{L} = q\sqrt{-\frac{\mu\kappa^2}{2E}}, \qquad \mathbf{L}^2 + \mathbf{B}^2 + 1 = q^2 - \frac{\mu\kappa^2}{2E} \tag{5}$$

The wave function ψ should not be thought of as an ordinary function, but a "*section*" [18]. In the $x_1x_2x_3$ space, in the basis $|H, \mathbf{L}^2, L_3>$, $\psi_{q,n,l,m}(\mathbf{r}) = R_{q,n,l}(r)Y_{q,l,m}(\theta,\phi)$, where

$$R_{q,n,l}(r) = C_{n,l} r^l e^{-\sqrt{-2\mu E_n}r}\ {}_1F_1(l + 1 - n; 2l + 2; 2\sqrt{-2\mu E_n}r) \tag{6}$$

is the radial wave function. $Y_{q,l,m}(\theta, \phi) = \Theta_{q,l,m}(\theta)\Phi_{q,m}(\phi)$ is the monopole harmonic, with

$$L_3\Phi_{q,m}(\phi) = m\Phi_{q,m}(\phi), \qquad [\Phi_{q,m}(\phi)]_a = e^{i(m+q)\phi}, \qquad (7)$$
$$[\Phi_{q,m}(\phi)]_b = e^{i(m-q)\phi}$$

where $[\Phi_{q,m}(\phi)]_a$ corresponds to region R_a, and $\psi_a = e^{2iq\phi}\psi_b$. The eigenenergy $E_n = -(\mu\kappa^2/2)(1/n^2)$, and $n = |q| + 1, |q| + 2, \ldots$. Obviously, when $q = 0$, all of the equations described above will reduce to the usual ones. In fact, the monopolar hydrogen atom contains all the analogous properties of the usual system. To our knowledge, connecting such an extended hydrogen atom to a 4D harmonic oscillator by the KS transformation has not been discussed in the literature. The purpose of this paper is to establish such a connection.

2. HYDROGEN OSCILLATOR CONNECTION BY THE KS TRANSFORMATION

To connect the monopolar $\mathbf{R}^3$ hydrogen atom [see Eq. (1)] to the $\mathbf{R}^4$ harmonic oscillator [see Eq. (21)], we first discuss the problem in the region R_a. The so-called KS transformation is

$$\begin{aligned} x_1 &= 2(u_1 u_3 - u_2 u_4), \\ x_2 &= 2(u_1 u_4 + u_2 u_3), \\ x_3 &= u_1^2 + u_2^2 - u_3^2 - u_4^2 \end{aligned} \qquad (8)$$

where x_i ($i = 1, 2, 3$) and u_α ($\alpha = 1, 2, 3, 4$) are the Cartesian coordinates of $\mathbf{R}^3$ and $\mathbf{R}^4$, respectively. Under the transformation $r = (x_1^2 + x_2^2 + x_3^2)^{1/2} = u^2$, x_i and u_α are usually realized by

$$x_1 = r \sin\theta \cos\phi, \qquad x_2 = r \sin\theta \sin\phi, \qquad x_3 = r\cos\theta \qquad (9)$$

and

$$u_1 = \sqrt{r}\cos\frac{\theta}{2}\cos\omega_1, \qquad u_2 = \sqrt{r}\cos\frac{\theta}{2}\sin\omega_1$$
$$u_3 = \sqrt{r}\sin\frac{\theta}{2}\cos\omega_2, \qquad u_4 = \sqrt{r}\sin\frac{\theta}{2}\sin\omega_2 \qquad (10)$$

with $\phi = \omega_1 + \omega_2$. However, since the KS transformation is ($u_1, u_2, u_3, u_4 \to x_1, x_2, x_3$), the degree of freedom in $\mathbf{R}^4$ is greater than that in $\mathbf{R}^3$ by one, and when we evaluate $\partial/\partial u_\alpha$ ($\alpha = 1, 2, 3, 4$), it is necessary to consider the fourth variable (denoted by T). Now, $\partial/\partial T$ will be related to a $U(1)$ magnetic monopole. As will be seen, without the monopole, $\partial\psi/\partial T = 0$ is just the constraint condition for the usual problem, and in that case we need not consider the fourth variable T. Taking the fourth variable T into account, we obtain

$$\frac{\partial}{\partial u_1} = 2\left(u_3 \frac{\partial}{\partial x_1} + u_4 \frac{\partial}{\partial x_2} + u_1 \frac{\partial}{\partial x_3}\right) + \frac{\partial T}{\partial u_1}\frac{\partial}{\partial T}$$

$$\frac{\partial}{\partial u_2} = 2\left(-u_4 \frac{\partial}{\partial x_1} + u_3 \frac{\partial}{\partial x_2} + u_2 \frac{\partial}{\partial x_3}\right) + \frac{\partial T}{\partial u_2}\frac{\partial}{\partial T}$$

$$\frac{\partial}{\partial u_3} = 2\left(u_1 \frac{\partial}{\partial x_1} + u_2 \frac{\partial}{\partial x_2} - u_3 \frac{\partial}{\partial x_3}\right) + \frac{\partial T}{\partial u_3}\frac{\partial}{\partial T}$$

$$\frac{\partial}{\partial u_4} = 2\left(-u_2 \frac{\partial}{\partial x_1} + u_1 \frac{\partial}{\partial x_2} - u_4 \frac{\partial}{\partial x_3}\right) + \frac{\partial T}{\partial u_4}\frac{\partial}{\partial T} \qquad (11)$$

which can be recast as

$$\frac{\partial}{\partial u_1} = 2i(u_3\pi_1 + u_4\pi_2 + u_1\pi_3 + u_2 S)$$

$$\frac{\partial}{\partial u_2} = 2i(-u_4\pi_1 + u_3\pi_2 + u_2\pi_3 - u_1 S)$$

$$\frac{\partial}{\partial u_3} = 2i(u_1\pi_1 + u_2\pi_2 - u_3\pi_3 - u_4 S)$$

$$\frac{\partial}{\partial u_4} = 2i(-u_2\pi_1 + u_1\pi_2 - u_4\pi_3 + u_3 S) \qquad (12)$$

where $\pi_i = p_i - eA_i$ $(i = 1, 2, 3)$, we have set $\hbar = c = 1$, and

$$u_2 S = -\frac{i}{2}\frac{\partial T}{\partial u_1}\frac{\partial}{\partial T} + e(u_3A_1 + u_4A_2 + u_1A_3)$$

$$-u_1 S = -\frac{i}{2}\frac{\partial T}{\partial u_2}\frac{\partial}{\partial T} + e(-u_4A_1 + u_3A_2 + u_2A_3)$$

$$-u_4 S = -\frac{i}{2}\frac{\partial T}{\partial u_3}\frac{\partial}{\partial T} + e(u_1A_1 + u_2A_2 - u_3A_3)$$

$$u_3 S = -\frac{i}{2}\frac{\partial T}{\partial u_4}\frac{\partial}{\partial T} + e(-u_2A_1 + u_1A_2 - u_4A_3) \qquad (13)$$

The inversion of Eqs. (12) is

$$\pi_1 = -\frac{i}{2}\frac{1}{u^2}\left(u_3 \frac{\partial}{\partial u_1} - u_4 \frac{\partial}{\partial u_2} + u_1 \frac{\partial}{\partial u_3} - u_2 \frac{\partial}{\partial u_4}\right)$$

$$\pi_2 = -\frac{i}{2}\frac{1}{u^2}\left(u_4 \frac{\partial}{\partial u_1} + u_3 \frac{\partial}{\partial u_2} + u_2 \frac{\partial}{\partial u_3} + u_1 \frac{\partial}{\partial u_4}\right)$$

$$\pi_3 = -\frac{i}{2}\frac{1}{u^2}\left(u_1\frac{\partial}{\partial u_1} + u_2\frac{\partial}{\partial u_2} - u_3\frac{\partial}{\partial u_3} - u_4\frac{\partial}{\partial u_4}\right)$$

$$S = -\frac{i}{2}\frac{1}{u^2}\left(u_2\frac{\partial}{\partial u_1} - u_1\frac{\partial}{\partial u_2} - u_4\frac{\partial}{\partial u_3} + u_3\frac{\partial}{\partial u_4}\right) \tag{14}$$

Equations (14) yield

$$[rS, \pi_i] = [rS, x_i] = 0, \qquad [\pi_i, \pi_j] = i\epsilon_{ijk}\frac{x_k}{r^2}S \qquad (i, j, k, = 1, 2, 3) \tag{15}$$

After comparing Eqs. (15) and (4), one obtains

$$S = q/r \tag{16}$$

Note that Eq. (16), as well as similar relations in this paper, are to be understood as acting on the wave function ψ of the system concerned. For $q = 0$, Eq. (15) reduces to the usual result, and the KS transformation connects the usual $\mathbf{R}^3$ hydrogen atom to an $\mathbf{R}^4$ harmonic oscillator with the constraint $S\psi = 0$.

From Eqs. (14) we get

$$\vec{\pi}^2 = -\frac{1}{4}\frac{1}{u^2}\sum_{\alpha=1}^{4}\frac{\partial^2}{\partial u_\alpha^2} - S^2 \tag{17}$$

substituting this into Eq. (1) gives for the Schrödinger equation

$$\left[-\frac{1}{8\mu}\frac{1}{u^2}\sum_{\alpha=1}^{4}\frac{\partial^2}{\partial u_\alpha^2} + \frac{1}{2\mu}\left(\frac{q^2}{r^2} - S^2\right) - \frac{\kappa}{r}\right]\psi = E\psi \tag{18}$$

Multiplying this by r, using $r = u^2$, and taking the constraint condition $(rS = q)\psi$ into account, leads to

$$\left[-\frac{1}{8\mu}\sum_{\alpha=1}^{4}\frac{\partial^2}{\partial u_\alpha^2} - Eu^2\right]\psi = \kappa\psi \tag{19}$$

This may be cast into the form of a Schrödinger equation for a four-dimensional harmonic oscillator after first stipulating that $E < 0$ (for bound motions) and making the definitions $m = 4\mu$, $\Omega = (-E/2\mu)^{1/2}$, and $\epsilon = \kappa$. We obtain

$$\left(-\frac{1}{2m}\sum_{\alpha=1}^{4}\frac{\partial^2}{\partial u_\alpha^2} + \frac{1}{2}m\Omega^2u^2\right)\psi = \epsilon\psi \tag{20}$$

or $\mathcal{H}_0\psi = \epsilon\psi$, with

$$\mathcal{H}_0 = -\frac{1}{2m}\sum_{\alpha=1}^{4}\frac{\partial^2}{\partial u_\alpha^2} + \frac{1}{2} m\Omega^2 u^2 \tag{21}$$

$\mathcal{H}_0$ and ϵ are the pseudo-Hamiltonian of a four-dimensional harmonic oscillator and the pseudo-energy eigenvalue, respectively. Consequently, the $\mathbf{R}^3$ monopolar hydrogen atom system is connected to the $\mathbf{R}^4$ harmonic oscillator with a monopole-dependent constraint (16) by the KS transformation.

To see the consistency of the constraint condition, we return to Eqs. (13). In the $x_1x_2x_3$ coordinates, $\mathbf{A}_a$ is expressed as

$$(A_1)_a = -\frac{g}{r}\tan\frac{\theta}{2}\sin\phi, \qquad (A_2)_a = \frac{g}{r}\tan\frac{\theta}{2}\cos\phi, \qquad (A_3)_a = 0 \tag{22}$$

Substituting Eqs. (10), (16), and (22) into Eq. (13), one obtains

$$\begin{aligned} \frac{i}{2}\frac{\partial T_a}{\partial u_1}\frac{\partial}{\partial T_a} &= -q\,\frac{u_2}{u_1^2 + u_2^2} \\ \frac{i}{2}\frac{\partial T_a}{\partial u_2}\frac{\partial}{\partial T_a} &= q\,\frac{u_1}{u_1^2 + u_2^2} \\ \frac{i}{2}\frac{\partial T_a}{\partial u_3}\frac{\partial}{\partial T_a} &= \frac{i}{2}\frac{\partial T_a}{\partial u_4}\frac{\partial}{\partial T_a} = 0 \end{aligned} \tag{23}$$

where T_a means discussing T in the region R_a. If we set $\omega_1 = \beta$, $\omega_2 = \phi - \beta$, in other words,

$$\beta = \arctan\frac{u_2}{u_1}, \qquad \phi = \arctan\frac{u_2}{u_1} + \arctan\frac{u_4}{u_3} \tag{24}$$

the solution is

$$T_a = \beta, \qquad \left(\frac{i}{2}\frac{\partial}{\partial T_a} = q\right)\psi \tag{25}$$

In region R_a, the KS transformation is understood as $(r, \theta, \phi, \beta \to r, \theta, \phi)$; since T_a is β, it is reasonable and acceptable to consider the fourth variable in Eq. (11).

After substituting Eqs. (8) and (14) into the first of Eqs. (3), we obtain

$$L_3 = -i\frac{\partial}{\partial\phi} - q + \sin^2\!\left(\frac{\theta}{2}\right)\left[-i\frac{\partial}{\partial\beta} + 2q\right] \tag{26}$$

whose eigenfunction is

$$\Phi_{q,m}(\phi, \beta) = e^{i(m+q)\phi}\, e^{-i2q\beta} \tag{27}$$

Obviously, $\Phi_{q,m}(\phi, \beta)$ differs from $[\Phi_{q,m}(\phi)]_a$ merely by a phase factor $e^{-i2q\beta}$, and L_3 becomes $(L_3)_a = -i\, \partial/\partial\phi - q$ when it is acted on by $\Phi_{q,m}(\phi, \beta)$. Since $[(i/2)\, \partial/\partial\beta = rS = q]\Phi_{q,m}(\phi, \beta)$, the constraint condition (16) is well understood.

A similar discussion can be given for region R_b. The corresponding equations and solutions are (by setting $\omega_1 = \phi - \gamma$, $\omega_2 = \gamma$)

$$\begin{aligned}
\frac{i}{2}\frac{\partial T_b}{\partial u_3}\frac{\partial}{\partial T_b} &= q\,\frac{u_4}{u_3^2 + u_4^2} \\
\frac{i}{2}\frac{\partial T_b}{\partial u_4}\frac{\partial}{\partial T_b} &= -q\,\frac{u_3}{u_3^2 + u_4^2} \\
\frac{i}{2}\frac{\partial T_b}{\partial u_1}\frac{\partial}{\partial T_b} &= \frac{i}{2}\frac{\partial T_b}{\partial u_2}\frac{\partial}{\partial T_b} = 0
\end{aligned} \tag{28}$$

and

$$T_b = \gamma = \arctan\frac{u_4}{u_3}, \qquad \left(\frac{i}{2}\frac{\partial}{\partial T_b} = -q\right)\psi \tag{29}$$

In this case, the constraint is understood as $[-(i/2)\, \partial/\partial\gamma = rS = q]\Phi_{q,m}(\phi, \gamma)$, where $\Phi_{q,m}(\phi, \gamma) = e^{i(m-q)\phi}\, e^{i2q\gamma}$.

In conclusion, the KS transformation is shown to connect a $U(1)$ monopolar hydrogen atom to a four-dimensional isotropic harmonic oscillator with a reasonable monopole-dependent constraint. The constraint $S = q/r$ is well understood when it acts on the wave function ψ, and it is related to $\mathbf{L} \cdot \mathbf{R} = q$. For the case without the monopole, i.e., $q = 0$, the constraint implies that the usual angular momentum vector and the usual PRL vector are orthogonal to each other, which is just the case in the usual Coulomb problem.

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