

The Kustaanheimo-Stiefel transformation applied to the hydrogen atom: using the constraint equation and resolving a wavefunction discrepancy

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1990 J. Phys. A: Math. Gen. 23 1519

(<http://iopscience.iop.org/0305-4470/23/9/016>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 129.252.86.83

The article was downloaded on 01/06/2010 at 10:06

Please note that [terms and conditions apply](#).

The Kustaanheimo–Stiefel transformation applied to the hydrogen atom: using the constraint equation and resolving a wavefunction discrepancy

E Cahill†

Department of Mathematical Physics, University College, Dublin 4, Ireland

Received 1 November 1989

Abstract. We show how explicit use of the constraint equation that arises when the Kustaanheimo–Stiefel transformation is applied to the hydrogen atom in \mathbf{R}^3 enables us to determine the wavefunctions for the constrained harmonic oscillator in \mathbf{R}^4 with the correct restriction on the quantum numbers in a direct and natural manner. We then highlight and resolve a discrepancy between the \mathbf{R}^4 oscillator wavefunctions produced by different authors by considering the measure to be used in \mathbf{R}^4 and the operator ordering in the quantised Hamiltonian.

Many approaches have been used to investigate the relationship between the non-relativistic hydrogen atom and the isotropic harmonic oscillator. For a review see Chen (1982) and Kibler *et al* (1986). One of the most popular approaches has been via the use of the ks transformation (Kustaanheimo and Stiefel 1965). This is a non-bijective mapping from rectangular Cartesian coordinates for \mathbf{R}^3 to rectangular Cartesians for \mathbf{R}^4 subject to a constraint.

When this transformation is applied to the hydrogen atom in \mathbf{R}^3 the constraint is manifest as a restriction on the oscillator quantum numbers. The usual procedure for determining this restriction is to compare the expressions for the energy eigenvalues for the oscillator and for the hydrogen atom and by demanding consistency of the two, the restriction can be obtained (Chen 1982). Here we demonstrate how this restriction arises naturally when we take the constraint into consideration.

Following Kennedy (1982) we use the ks transformation from \mathbf{R}^3 to \mathbf{R}^4 in the form

$$\begin{pmatrix} dx_1 \\ dx_2 \\ dx_3 \\ 0 \end{pmatrix} = 2 \begin{pmatrix} q_1 & -q_2 & -q_3 & q_4 \\ q_2 & q_1 & -q_4 & -q_3 \\ q_3 & q_4 & q_1 & q_2 \\ q_4 & -q_3 & q_2 & -q_1 \end{pmatrix} \begin{pmatrix} dq_1 \\ dq_2 \\ dq_3 \\ dq_4 \end{pmatrix} \quad (1)$$

and we take as our self-adjoint hydrogen Hamiltonian:

$$H = \frac{1}{8m} \frac{1}{q} p^2 \frac{1}{q} - \frac{e^2}{q^2}.$$

† Present address: National Grid, Research and Development Centre, Kelvin Avenue, Leatherhead, Surrey KT22 7ST, UK.

The constraint arising from the last row of (1) becomes (Kennedy 1982):

$$q_1 p_4 - q_2 p_3 + q_3 p_2 - q_4 p_1 = 0. \quad (2)$$

Next we quantise the system by making the usual assignments

$$p_k \rightarrow -i\hbar \frac{\partial}{\partial q_k}.$$

In order to quantise the constraint equation (2) we do not treat it as an operator identity but instead following Dirac (1964) we interpret it as a restriction on allowed energy states. Acceptable wavefunctions must be in the kernel of the operator on the left of (2):

$$\left(q_1 \frac{\partial}{\partial q_4} - q_2 \frac{\partial}{\partial q_3} + q_3 \frac{\partial}{\partial q_2} - q_4 \frac{\partial}{\partial q_1} \right) \psi = 0. \quad (3)$$

We now introduce polar coordinates for \mathbf{R}^4 (Chen 1980)

$$\begin{aligned} q_1 &= R \cos \omega \sin \eta \\ q_4 &= R \cos \omega \cos \eta \\ q_2 &= R \sin \omega \sin \xi \\ q_3 &= R \sin \omega \cos \xi \end{aligned} \quad (4)$$

and the Schrödinger equation becomes:

$$\begin{aligned} \frac{-\hbar^2}{8m} \left[\frac{1}{R^4} \frac{\partial}{\partial R} \left(R^3 \frac{\partial}{\partial R} \left(\frac{\psi}{R} \right) \right) + \frac{1}{R^4} \left(\frac{1}{\cos^2 \omega} \frac{\partial^2 \psi}{\partial \eta^2} + \frac{1}{\sin^2 \omega} \frac{\partial^2 \psi}{\partial \xi^2} \right) \right. \\ \left. + \frac{1}{R^4 \cos \omega \sin \omega} \frac{\partial}{\partial \omega} \left(\cos \omega \sin \omega \frac{\partial \psi}{\partial \omega} \right) \right] - \frac{e^2}{R^2} \psi = E\psi. \end{aligned} \quad (5)$$

The constraint (3) assumes the simple form

$$\left(\frac{\partial}{\partial \eta} - \frac{\partial}{\partial \xi} \right) \psi = 0. \quad (6)$$

If we now let

$$\psi(R, \eta, \xi, \omega) = X(R)H(\eta)G(\xi)W(\omega) \quad (7)$$

and separate the variables we obtain

$$\frac{-\hbar^2}{8m} \frac{1}{R^4} \frac{d}{dR} \left[R^3 \frac{d}{dR} \left(\frac{X}{R} \right) \right] - \left(\frac{e^2}{R^2} + \frac{\lambda}{R^4} \right) X = EX \quad (8)$$

$$H'' + \mu H = 0 \quad (9)$$

$$G'' + \nu G = 0 \quad (10)$$

$$\tan \omega \frac{d}{d\omega} (\sin 2\omega W') - 2 \left(\nu + \mu \tan^2 \omega + \frac{8m}{\hbar^2} \lambda \sin^2 \omega \right) W = 0. \quad (11)$$

Angular equations. Next we use the constraint to restrict the class of acceptable wavefunctions. Using (7) and separation of the variables in (6) yields

$$H(\eta) = A \exp(\kappa\eta) \quad G(\xi) = B \exp(-\kappa\xi). \quad (12)$$

From (9) and (10) we must have (Schiff 1968)

$$\mu = m_1^2 \quad \nu = m_2^2 \quad m_1, m_2 \in \mathbb{Z} \tag{13}$$

and (13) implies

$$m_1 = m_2 \equiv m \tag{14}$$

and

$$\kappa = \pm im. \tag{15}$$

Therefore the constraint has enabled us to determine the restriction on the oscillator quantum numbers directly.

If we now let

$$\theta = 2\omega \quad \text{and} \quad \Theta(\theta) = W(\omega)$$

and use (14), then (11) can be reduced to

$$\frac{1}{\sin \theta} \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta} \right) - \left(\frac{m^2}{\sin^2 \theta} + \frac{2m\lambda}{\hbar^2} \right) \Theta = 0. \tag{16}$$

This is the θ for hydrogen and so we must have (Schiff 1968)

$$\lambda = \frac{-\hbar^2}{2m} l(l+1) \tag{17}$$

$$W(\omega) = P_l^m(\cos 2\omega). \tag{18}$$

The normalised angular component of the constrained oscillator wavefunction is then

$$H(\eta)G(\xi)W(\omega) = Y_{lm}(2\omega, \eta + \xi). \tag{19}$$

Radial equation. If we make the substitutions (Cizek and Paldus 1977)

$$r = R^2 \quad \Lambda(r) = \frac{1}{R} X(R) \tag{20}$$

then the oscillator radial equation reduces to the normal hydrogen radial equation:

$$\frac{-\hbar^2}{2m} \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d\Lambda}{dr} \right) - \left(\frac{e^2}{r} - \frac{\hbar^2}{2m} l(l+1) \right) \Lambda = E\Lambda. \tag{21}$$

Therefore the complete oscillator wavefunction which satisfies the constraint is

$$\psi_{nlm}(R, \omega, \eta, \xi) = N \exp(-\frac{1}{2}\sigma) \sigma^{l+1/2} L_{n+l}^{2l+1}(\sigma) Y_{lm}(2\omega, \eta + \xi) \tag{22}$$

where $\sigma = (2me^2/\hbar^2 n)R^2$ and $L_{n+l}^{2l+1}(\sigma)$ are as defined in Schiff (1968) and N is a normalisation constant.

A measure for R^4 . The correspondence with the usual hydrogen wavefunctions is obvious, the only discrepancy being the occurrence of the factor $\sigma^{1/2}$. This factor does not occur in the wavefunctions as given by Chen (1982). However, he notes the need to introduce an artificial volume element for R^4 for his wavefunctions. This discrepancy is resolved when consideration is given to the measure to be used when integrating over R^4 . Kennedy (1982) transformed the classical hydrogen atom in R^3 to R^4 and then quantised it, so the appropriate measure is the ‘natural’ volume element for R^4 :

$$dV = dq_1 dq_2 dq_3 dq_4.$$

His ordering for the kinetic component of the Hamiltonian, $(1/q)p^2(1/q)$, is self-adjoint with respect to this measure (Cahill 1988).

However, in the works of Chen (1982), Kibler *et al* (1986) and Davtyan *et al* (1987) the hydrogen atom is first quantised in \mathbf{R}^3 and then the resulting differential equation is mapped to \mathbf{R}^4 via the KS transformation. So the appropriate measure is the transformed \mathbf{R}^3 volume element which is (Cahill 1988)

$$dV' = q^2 dV.$$

When transforming the Schrödinger equation from \mathbf{R}^3 to \mathbf{R}^4 the Laplacian transforms as

$$\nabla_3^2 \rightarrow \frac{1}{q^2} \nabla_4^2$$

and so formally transforming the quantised system is equivalent to quantising in \mathbf{R}^4 with the operator ordering

$$\frac{1}{q^2} p^2$$

and this ordering is self-adjoint with respect to

$$q^2 dV.$$

These distinct approaches give rise to radial wavefunctions which differ by a factor of q . However they give rise to the same probabilities when we use the appropriate measure

$$|X(q)|^2 q^2 dV = |qX(q)|^2 dV.$$

Acknowledgment

I am grateful to Dr J Kennedy for his advice during the preparation of this paper.

References

- Cahill E 1988 Factorisation and Supersymmetry in Quantum Mechanics *MSc thesis* University College, Dublin
- Chen A C 1980 *Phys. Rev. A* **22** 333
- 1982 *J. Math. Phys.* **23** 412-6
- Cizek J and Paldus J 1977 *Int. J. Quantum Chem.* **12** 875-96
- Davtyan L S, Mardoyan L G, Pogosyan G S, Sissakian A N and Ter-Antonyan V M 1987 *J. Phys. A: Math. Gen.* **20** 6121-5
- Dirac P A M 1964 *Lectures on Quantum Mechanics* (New York: Belfer)
- Kennedy J 1982 *Proc. R. Irish Acad. A* **82** 1-8
- Kibler M, Ronveaux A and Negadi T 1986 *J. Math. Phys.* **27** 1541-8
- Kustaanheimo P and Stiefel E 1965 *J. Reine Angew. Math.* **218** 204-19
- Schiff L I 1968 *Quantum Mechanics* (New York: McGraw-Hill) p 76-94