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The hydrogen atom and the four-dimensional harmonic oscillator

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Abstract. Through the introduction of two complex stereographic variables it is shown that the Schrödinger equation for the bound states of hydrogen reduces to the wave equation for two coupled two-dimensional harmonic oscillators. The wavefunctions obtained by this means are the same as those which arise using parabolic coordinates.

1. Introduction

It has long been known that the degeneracy of the bound states of the non-relativistic hydrogen atom may be described in terms of a dynamical symmetry group isomorphic to $O(4)$. Schwinger (1964) used this symmetry in the momentum representation to derive Green's function for the Coulomb field and a fuller discussion of the application of group theory to the hydrogen atom was given by Bander and Itzykson (1966). More recent work has been based on a coordinate transformation introduced for the corresponding classical problem by Kustaanheimo and Stiefel (1965) as a generalisation of the parabolic coordinates due to Levi-Civita. The κs transformation was used by Boiteux (1972, 1973) to show that the bound states of the hydrogen atom correspond to the energy eigenstates of a four-dimensional isotropic oscillator subject to a constraint. Kennedy (1982) applied to this problem the Dirac method for dealing with constraints and showed in detail how the constraint equation leads to the energy levels of hydrogen with the correct degree of degeneracy. The κs transformation was also exploited by Duru and Kleinert (1979) in carrying through for the first time the Feynman path integral method to calculate the Coulomb Green's function. This calculation was much improved by Ho and Inomata (1982).

It is easy to show that the two-dimensional Coulomb wave equation is mapped into the equation for a two-dimensional harmonic oscillator by the introduction of plane parabolic coordinates. The transformation from cartesian x, y to plane parabolic coordinates λ, μ may be expressed in complex form by $x + iy = \frac{1}{2}(\lambda + i\mu)^2$, and was used by Barut and Duru (1973) to relate the two-dimensional Kepler and oscillator interpretations of a composite relativistic system within $SO(3, 2)$. In a later paper Barut, Schneider and Wilson (1979) used a coordinate transformation involving two complex variables to relate the three-dimensional Kepler and four-dimensional harmonic oscillator interpretations of a composite relativistic object in $SO(4, 2)$. They showed that their transformation is a generalisation of the Kustaanheimo–Stiefel transformation.

In the present paper we show that the bsw transformation expressed as a generalised stereographic coordinate transformation when applied directly to Schrödinger's

equation for the bound states of hydrogen leads to the wave equation for an isotropic four-dimensional harmonic oscillator with a constraint condition. The formalism shows that the oscillator with constraint may be regarded as two two-dimensional oscillators subject to the condition that their angular momenta are equal and opposite. Following this simple interpretation of the constraint condition and using the wavefunctions for a two-dimensional harmonic oscillator involving associated Laguerre polynomials, the energy levels and wavefunctions for hydrogen are easily deduced. The somewhat involved procedure used by Kennedy (1982) in applying the constraint condition to wavefunctions expressed as products of four Hermite polynomials is thereby avoided. The wavefunctions are the same as those which arise by solving Schrödinger's equation in (rotational) parabolic coordinates. As is well known, these wavefunctions are the simultaneous eigenfunctions of the energy, the z component of the angular momentum and the z component of the Runge-Lenz vector.

2. Transformation and solution of the wave equation

The energy levels and wavefunctions for the bound states of hydrogen are given by the solution of Schrödinger's equation

$$(-\hbar^2/2\mu)\nabla^2 - e^2/r \psi = E\psi, \quad E < 0, \quad (1)$$

which may be rewritten as

$$(4\nabla^2 + \lambda/r - \alpha^4)\psi = 0, \quad (2)$$

where

$$\lambda = 8/a, \quad \alpha^4 = -8E/e^2 a, \quad a = \hbar^2/\mu e^2. \quad (3)$$

Now introduce two complex variables ζ_A and ζ_B , and consider the relations

$$x + iy = 2\zeta_A \bar{\zeta}_B, \quad z = \zeta_A \bar{\zeta}_A - \zeta_B \bar{\zeta}_B, \quad (4)$$

from which it follows that

$$r = (x^2 + y^2 + z^2)^{1/2} = \zeta_A \bar{\zeta}_A + \zeta_B \bar{\zeta}_B. \quad (5)$$

For any chosen pair of values for ζ_A and ζ_B these relations determine a unique set of values for the cartesian coordinates x, y, z . The converse is not true. In particular, arbitrary but equal changes in the arguments of ζ_A and ζ_B leave x, y, z unchanged. Writing

$$\sigma = \arg \zeta_A \zeta_B, \quad (6)$$

equation (4) may be solved to give ζ_A and ζ_B in terms of σ and the spherical polar coordinates defined in the usual way in x, y, z space:

$$\zeta_A = r^{1/2} \cos(\tfrac{1}{2}\theta) e^{i(\sigma+\phi)/2}, \quad \zeta_B = r^{1/2} \sin(\tfrac{1}{2}\theta) e^{i(\sigma-\phi)/2}. \quad (7)$$

Thus for any given choice of x, y, z the complex variables ζ_A and ζ_B are determined to within an arbitrary value for the angle σ . This also follows from the fact that the group $U(2)$ of unitary linear transformations of the complex variables ζ_A and ζ_B generates through relations (4) the group $O(3)$ of rotations in x, y, z space, but that each member of $O(3)$ determines a member of $U(2)$ only to within an arbitrary factor of modulus unity.

We next express Schrödinger's equation for the hydrogen atom in terms of the new variables ζ_A, ζ_B . It is straightforward to show that

$$r\nabla^2\psi(x, y, z) = (\partial_A\partial_{\bar{A}} + \partial_B\partial_{\bar{B}})\psi, \quad (8)$$

where $\partial_A = \partial/\partial\zeta_A$ and similarly for $\partial_{\bar{A}}, \partial_B$ and $\partial_{\bar{B}}$. Then (2) becomes

$$[4\partial_A\partial_{\bar{A}} + 4\partial_B\partial_{\bar{B}} + \lambda - \alpha^4(\zeta_A\bar{\zeta}_A + \zeta_B\bar{\zeta}_B)]\psi = 0. \quad (9)$$

Clearly the wavefunction $\psi(x, y, z)$ when expressed as a function of ζ_A and ζ_B is independent of σ , so we must also have

$$\partial\psi/\partial\sigma = 0. \quad (10)$$

This is equivalent to the requirement that

$$(\bar{\zeta}_A\partial_{\bar{A}} - \zeta_A\partial_A)\psi = -(\bar{\zeta}_B\partial_{\bar{B}} - \zeta_B\partial_B)\psi. \quad (11)$$

Equations (9) and (11) are together equivalent to Schrödinger's equation (1) for hydrogen. But (9) is the wave equation for a four-dimensional harmonic oscillator. To see this more easily write

$$\zeta_A = q_1 + iq_2, \quad \zeta_B = q_3 + iq_4, \quad (12)$$

when (9) becomes

$$[\partial_1^2 + \partial_2^2 + \partial_3^2 + \partial_4^2 + \lambda - \alpha^4(q_1^2 + q_2^2 + q_3^2 + q_4^2)]\psi = 0, \quad (13)$$

where $\partial_i = \partial/\partial q_i$. This is the equation for an oscillator with frequency ω and energy ε given by

$$\alpha^2 \equiv (-8E/e^2a)^{1/2} = \mu\omega/\hbar, \quad \lambda \equiv 8/a = 2\mu\varepsilon/\hbar^2. \quad (14)$$

Condition (11) becomes

$$(q_1\partial_2 - q_2\partial_1)\psi = -(q_3\partial_4 - q_4\partial_3)\psi. \quad (15)$$

This means that the four-dimensional oscillator may be regarded as two two-dimensional oscillators whose angular momenta must always be equal and opposite. Writing $\psi = \psi_A(q_1, q_2)\psi_B(q_3, q_4)$ equation (13) separates to give

$$(\partial_1^2 + \partial_2^2 + \lambda_A - \alpha^4(q_1^2 + q_2^2))\psi_A = 0 \quad (16)$$

where $\lambda_A = 2\mu\varepsilon_A/\hbar^2$, with a similar equation for ψ_B so that

$$\lambda = \lambda_A + \lambda_B. \quad (17)$$

The simultaneous eigenfunctions of the energy and angular momentum for oscillator A are

$$\psi_{A n_1 l_1} = C_{n_1 l_1} (\zeta_A/\bar{\zeta}_A)^{l_1/2} (\alpha^2 \zeta_A \bar{\zeta}_A)^{|l_1|/2} \exp(-\frac{1}{2}\alpha^2 \zeta_A \bar{\zeta}_A) L_{n_1+|l_1|}^{|l_1|}(\alpha^2 \zeta_A \bar{\zeta}_A), \quad (18)$$

where $l_1 = 0, \pm 1, \pm 2, \dots$; $n_1 = 0, 1, 2, \dots$; $L_{n_1+|l_1|}^{|l_1|}$ are the associated Laguerre polynomials and $C_{n_1 l_1}$ are constants. The corresponding eigenvalues for the energy ε_A and angular momentum L_A are:

$$\varepsilon_{A n_1 l_1} = \hbar\omega(2n_1 + |l_1| + 1) = \hbar^2 \lambda_{A n_1 l_1} / 2\mu, \quad L_{A n_1 l_1} = l_1 \hbar. \quad (19)$$

The eigenfunctions $\psi_{B n_2 l_2}$ and eigenvalues for oscillator B are given by similar expressions with n_2, l_2, ζ_B replacing n_1, l_1 and ζ_A . Condition (15) requires that

$l_1 = -l_2 = l$ (say) so solutions of (9) and (11) are given by

$$\psi_{n_1 n_2 l} = \psi_{A n_1 l}(\zeta_A, \bar{\zeta}_A) \psi_{B n_2 - l}(\zeta_B, \bar{\zeta}_B), \quad (20)$$

with λ taking the values

$$\lambda_{n_1 n_2 l} = 4\alpha^2(n_1 + n_2 + |l| + 1). \quad (21)$$

These expressions must also give the energy eigenfunctions and eigenvalues for the hydrogen atom. From (18) and (20) using (7), the wavefunctions are:

$$\psi_{n_1 n_2 l} = K_{n_1 n_2 l} e^{i l \phi} (uv)^{|l|/2} \exp[-\frac{1}{2}(u+v)] L_{n_1+|l|}^{|l|}(u) L_{n_2+|l|}^{|l|}(v) \quad (22)$$

where

$$u = \alpha^2 \zeta_A \bar{\zeta}_A = \alpha^2 r \cos^2(\theta/2), \quad v = \alpha^2 \zeta_B \bar{\zeta}_B = \alpha^2 r \sin^2(\theta/2), \quad (23)$$

and where $K_{n_1 n_2 l}$ are constants. Equations (14) and (21) give for α^2 and the energy the values

$$\alpha^2 = 2/Na, \quad E_{n_1 n_2 l} = -e^2/2aN^2, \quad (24)$$

where $N = n_1 + n_2 + |l| + 1$, and where $n_1 = 0, 1, 2, \dots$; $n_2 = 0, 1, 2, \dots$; $l = 0, \pm 1, \pm 2, \dots$. These expressions constitute the well known solution for the hydrogen atom obtained by using parabolic coordinates ξ and η defined by

$$x = (\xi\eta)^{1/2} \cos \phi, \quad y = (\xi\eta)^{1/2} \sin \phi, \quad z = \frac{1}{2}(\xi - \eta) \quad (25)$$

(see Condon and Shortley 1953). Relations (25) are equivalent to

$$\xi = 2r \cos^2(\theta/2) = 2|\zeta_A|^2, \quad \eta = 2r \sin^2(\theta/2) = 2|\zeta_B|^2. \quad (26)$$

Note that the complex stereographic transformation (4) reduces to the transformation to parabolic coordinates (25) when (26) is used to express formulae (7) for the complex variables as

$$\zeta_A = (\xi/2)^{1/2} e^{i(\sigma+\phi)/2}, \quad \zeta_B = (\eta/2)^{1/2} e^{i(\sigma-\phi)/2}. \quad (27)$$

The wavefunctions $\psi_{n_1 n_2 l}$ are known to be the simultaneous eigenfunctions of the energy, the angular momentum about Oz and the z component of the Runge-Lenz vector

$$\mathbf{M} = (1/2\mu)(\mathbf{p} \times \mathbf{L} - \mathbf{L} \times \mathbf{p}) - (e^2/r)\mathbf{r}. \quad (28)$$

(In the classical case \mathbf{M} is directed along the major axis of an elliptical orbit). In terms of the variables ζ_A and ζ_B the operator M_z is given by

$$M_z = (e^2 a/r)(|\zeta_B|^2 \partial_A \partial_{\bar{A}} - |\zeta_A|^2 \partial_B \partial_{\bar{B}} - a^{-1}(|\zeta_A|^2 + |\zeta_B|^2)). \quad (29)$$

From the preceding formulae it is straightforward to show that

$$M_z \psi_{n_1 n_2 l} = [e^2(n_2 - n_1)/N] \psi_{n_1 n_2 l}. \quad (30)$$

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