

On the connection between the hydrogen atom and the harmonic oscillator:
the continuum case

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Abstract. The connection between a three-dimensional nonrelativistic hydrogen atom with positive energy and a four-dimensional isotropic harmonic oscillator with repulsive potential is established by applying Jordan-Schwinger boson calculus to the algebra of the Laplace-Runge-Lenz-Pauli vector. The spectrum generating group $SO(4,2)$ both for the bound and free states of the three-dimensional hydrogen atom arises as a quotient of the group $Sp(8, R)$ associated to a four-dimensional isotropic harmonic oscillator with constraint.

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1. Introduction.

The connection between the hydrogen atom and the harmonic oscillator traces back to the early days of quantum mechanics. A correspondence between these two basic quantification cases was known to Schrödinger (1940) and probably also to Schwinger (cf. McIntosh 1959). More recently, the hydrogen-oscillator connection has been taken again. A link between the hydrogen atom and the harmonic oscillator was established for the corresponding radial Schrödinger wave equations (Bergmann and Frishman 1965). Furthermore, a connection between the \mathbb{R}^3 hydrogen atom and a \mathbb{R}^4 isotropic harmonic oscillator with constraint, or equivalently a coupled pair of \mathbb{R}^2 isotropic harmonic oscillators, has been investigated more or less independently by various people in the recent years. More specifically, such a connection has been worked out mainly in the case of the discrete spectrum ($E < 0$) of the \mathbb{R}^3 hydrogen atom and was set up by using the squared parabolic coordinates (Ravndal and Toyoda 1967) and by using implicitly (Ikeda and Miyachi 1970, Chen 1980, Iwai 1982) or explicitly (Boiteux 1972, Barut et al 1979) the so-called Kustaanheimo-Stiefel transformation, a $\mathbb{R}^4 \rightarrow \mathbb{R}^3$ surjection (corresponding to a $S^3 \times \mathbb{R}^+ \rightarrow S^2 \times \mathbb{R}^+$ Hopf fibration) initially introduced for the regularization of the \mathbb{R}^3 Kepler problem (Kustaanheimo and Stiefel 1965). Further, the hydrogen-oscillator connection for the discrete spectrum ($E < 0$) has been recently obtained from the Pauli $SO(4)$ equations of the \mathbb{R}^3 hydrogen atom and the Jordan-Schwinger boson calculus (Kibler and Négadi 1983).

2. A preliminary result.

We shall deal in this paper with the continuous spectrum ($E > 0$) of the \mathbb{R}^3 hydrogen atom, a problem that was briefly touched upon by Barut et al (1979). We first recall (cf. Boiteux 1972) that the complete Schrödinger equation for a \mathbb{R}^3 hydrogenlike atom may be transformed via the Kustaanheimo-Stiefel transformation into

$$-\frac{\hbar^2}{2\mu} \sum_{j=1}^4 \frac{\partial^2}{\partial u_j^2} - 4E \sum_{j=1}^4 u_j^2 = 4Ze^2 \quad (1)$$

accompanied with a constraint condition ; in equation (1), Ze denotes the nucleus charge and μ the reduced mass of the hydrogenlike atom under

consideration. Therefore, in the case where $E > 0$, we may rewrite equation (1) as

$$-\frac{\hbar^2}{2\mu} \sum_{j=1}^4 \frac{\partial^2}{\partial u_j^2} - \frac{1}{2} \mu \omega^2 \sum_{j=1}^4 u_j^2 = \mathcal{E}, \quad (2)$$

where ω and \mathcal{E} are defined by

$$\begin{aligned} 4E &= \frac{1}{2} \mu \omega^2 \\ 4Ze^2 &= \mathcal{E}. \end{aligned} \quad (3)$$

Equation (2) is the Schrödinger equation for a \mathbb{R}^4 isotropic harmonic oscillator with a negative potential energy, the spectrum of which is clearly continuous. We thus obtain the result (see also Barut et al 1979) that there exists a correspondence between the scattering states ($E > 0$) of the \mathbb{R}^3 hydrogen atom and states of a \mathbb{R}^4 isotropic harmonic oscillator with a repulsive potential. The aim of this paper is to obtain and to further precise the just mentioned result without making use any longer of the Kustaanheimo-Stiefel transformation. The approach followed in this work is based on the Pauli $SO_0(3,1)$ equations relative to the continuous spectrum of the \mathbb{R}^3 hydrogen atom and the Jordan-Schwinger boson calculus. The merit of our approach is twofold: it allows us to easily introduce the spectral group $SO(4,2)$ of the \mathbb{R}^3 hydrogen atom (as seen below) and it seems to be (although not easily) extendable to higher-dimensional hydrogen atoms while such an extension is not possible through an à la Kustaanheimo-Stiefel transformation because of a famous result of Hurwitz (see Kustaanheimo and Stiefel 1965).

3. The main results.

We start from the two equations (Pauli 1926)

$$\vec{L} \cdot \vec{M} = \vec{M} \cdot \vec{L} = 0 \quad (4)$$

and

$$M^2 - (Ze^2)^2 = (2E/\mu) (\vec{L}^2 + \hbar^2) \quad (5)$$

relative to a R^3 hydrogenlike atom. In equations (4) and (5), \vec{M} stands for the Laplace-Runge-Lenz-Pauli operator and \vec{L} for the angular momentum operator. In the case of the free states ($E > 0$), by taking

$$\vec{B} = (\mu/2E)^{1/2} \vec{M}, \quad (6)$$

equations (4) and (5) specialize to

$$\vec{L} \cdot \vec{B} = \vec{B} \cdot \vec{L} = 0 \quad (7)$$

and

$$\vec{L}^2 - \vec{B}^2 + \hbar^2 = -(\mu/2E)(Ze^2)^2. \quad (8)$$

In addition, it is well-known that $\vec{L} (L_1, L_2, L_3)$ and $\vec{B} (B_1, B_2, B_3)$ span the Lie algebra of the Lorentz group $SO_0(3, 1)$, i. e.

$$[L_j, L_k] = i\hbar \epsilon_{jkl} L_l, \quad [L_j, B_k] = i\hbar \epsilon_{jkl} B_l, \quad [B_j, B_k] = -i\hbar \epsilon_{jkl} L_l. \quad (9)$$

A decisive point of this work amounts to finding a boson realization of the commutation relations (9). We shall take the following bilinear realization

$$\left. \begin{aligned} L_j &= (a^\dagger \sigma_j a + b^\dagger \sigma_j b) \hbar/2 \\ B_j &= (a^\dagger \sigma_j C \tilde{b}^\dagger - \tilde{a} C \sigma_j b) \hbar/2 \end{aligned} \right\} j = 1, 2, 3 \quad (10)$$

$$a = \begin{bmatrix} a_1 \\ a_2 \end{bmatrix}, \quad b = \begin{bmatrix} a_3 \\ a_4 \end{bmatrix}, \quad C = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix},$$

where σ_j ($j = 1, 2, 3$) are the standard Pauli matrices and where a_j and a_j^\dagger ($j = 1, 2, 3, 4$) are annihilation and creation Bose operators. [In passing we note in view of preparing the result below concerning $SO(4, 2)$ that the thirty-six possible bilinear forms of a_j and a_j^\dagger

($j = 1, 2, 3, 4$) span the Lie algebra of the symplectic group $Sp(8, R)$.] Then, we introduce equations (10) into equations (7) and (8). As a result, equation (7) yields

$$(a_1^+ a_1 + a_2^+ a_2 - a_3^+ a_3 - a_4^+ a_4)(a_1^+ a_4^+ + a_1 a_4 - a_2^+ a_3^+ - a_2 a_3) = 0 \quad (11)$$

and equation (8) leads to

$$(a_1^+ a_1 + a_2^+ a_2 - a_3^+ a_3 - a_4^+ a_4)^2 - (a_1^+ a_4^+ + a_1 a_4 - a_2^+ a_3^+ - a_2 a_3)^2 = -2\mu (Ze^2)^2 / (Eh^2). \quad (12)$$

(Equations (11) and (12), as well as related equations, are of course understood to be taken modulo their action on a given state vector ψ .) On account of the fact that the two factors in equation (11) commute, the bosonized expressions (11) and (12) can be combined to give the solution

$$a_1^+ a_1 + a_2^+ a_2 - a_3^+ a_3 - a_4^+ a_4 = 0 \quad (13)$$

and

$$(a_1^+ a_4^+ + a_1 a_4 - a_2^+ a_3^+ - a_2 a_3)^2 = 2\mu (Ze^2)^2 / (Eh^2). \quad (14)$$

We now show that equation (14) is amenable to a form that parallels the one of equation (2). By transforming the a_j and a_j^+ ($j = 1, 2, 3, 4$) defined on \mathbb{C}^4 into the Q_j and P_j ($j = 1, 2, 3, 4$) defined on $\mathbb{R}^4 \times \mathbb{R}^4$ owing to

$$Q_j = (2h/\mu\omega)^{1/2} (a_j + a_j^+)/2, \quad P_j = (2h\mu\omega)^{1/2} (a_j - a_j^+)/2i, \quad (15)$$

equation (14) reads

$$\frac{1}{2\mu} P_1 P_4 - \frac{1}{2} \mu\omega^2 Q_1 Q_4 - \frac{1}{2\mu} P_2 P_3 + \frac{1}{2} \mu\omega^2 Q_2 Q_3 = \omega(\mu/2E)^{1/2} Ze^2. \quad (16)$$

An evident canonical transformation

$\left\{ P_j, Q_j : j = 1, 2, 3, 4 \right\} \rightarrow \left\{ P_j', Q_j' : j = 1, 2, 3, 4 \right\}$ allows us to finally obtain

$$\frac{1}{2\mu} \sum_{j=1}^4 P_j'^2 - \frac{1}{2} \mu\omega^2 \sum_{j=1}^4 Q_j'^2 = \omega (2\mu/E)^{1/2} Ze^2, \quad (17)$$

to be compared with equation (2).

We thus end up with the result that the continuum states of a \mathbb{R}^3 hydrogen atom are connected with continuum states of a \mathbb{R}^4 isotropic harmonic oscillator with negative potential energy [cf. equation (17)] accompanied with a constraint condition [cf. equation (13)]. It is to be mentioned that the approach developed above for the scattering states of the \mathbb{R}^3 hydrogen atom can be also applied to the more familiar case of the bound states (Kibler and Négadi 1982). It is thus possible to obtain the known result that, in the case of the discrete spectrum, the \mathbb{R}^3 hydrogen atom problem is equivalent to the problem of a \mathbb{R}^4 isotropic harmonic oscillator with constraint and, even more precisely, to the problem of a coupled pair of \mathbb{R}^2 isotropic harmonic oscillators. We would like to mention the result that the constraint obtained in the discrete case (Kibler and Négadi 1982) is identical to the one obtained here in the continuous case [cf. equation (13)]. As a last result, we note that the introduction of the constraint given by equation (13) into the Lie algebra of the symplectic group $Sp(8, \mathbb{R})$ spanned by the set $\left\{ a_j^\dagger a_k^\dagger, a_j^\dagger a_k, a_j a_k : j \text{ and } k = 1, 2, 3, 4 \right\}$ gives rise to an under constraint Lie algebra that is indeed isomorphic to the Lie algebra of the pseudo-unitary group $SU(2, 2)$. The latter results are in agreement with the fact that the conformal group $SO(4, 2)$, locally isomorphic to $SU(2, 2)$, turns out to be the spectral (dynamical) group of the \mathbb{R}^3 hydrogen atom both for the bound and scattering states.

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