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

Maurice Kibler† and Tidjani Négadi‡

† Institut de Physique Nucléaire (et IN2P3), Université Claude Bernard Lyon-1, 43 Bd du 11 Novembre 1918, 69622 Villeurbanne Cedex, France

‡ Départment de Physique, Institut des Sciences Exactes, Université d'Oran, Es-Sénia, Oran, Algérie

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Abstract. The connection between a three-dimensional non-relativistic 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.

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 revived. 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 an $\mathbb{R}^4$ 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 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, an $\mathbb{R}^4 \to \mathbb{R}^3$ surjection (corresponding to an $S^3 \times \mathbb{R}^+ \to S^2 \times \mathbb{R}^+$ Hopf fibration) initially introduced for the regularisation 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 an $\mathbb{R}^3$ hydrogen-like atom may be transformed via the Kustaanheimo–Stiefel transformation into

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

accompanied by a constraint condition; in equation (1), Ze denotes the nucleus charge and μ the reduced mass of the hydrogen-like atom under consideration. Therefore, for $E > 0$, we may rewrite equation (1) as

$$-\frac{\hbar^2}{2\mu}\sum_{j=1}^{4}\frac{\partial^2}{\partial u_j^2}-\tfrac{1}{2}\mu\omega^2\sum_{j=1}^{4}u_j^2=\mathscr{E}, \tag{2}$$

where ω and $\mathscr{E}$ are defined by

$$4E=\tfrac{1}{2}\mu\omega^2, \qquad 4Ze^2=\mathscr{E}. \tag{3}$$

Equation (2) is the Schrödinger equation for an $\mathbb{R}^4$ 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 a correspondence exists between the scattering states ($E > 0$) of the $\mathbb{R}^3$ hydrogen atom and states of an $\mathbb{R}^4$ isotropic harmonic oscillator with a repulsive potential. The aim of this paper is to obtain and to make precise this result without making use 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 easily to 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 a Kustaanheimo–Stiefel-type 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)

$$\boldsymbol{L}\cdot\boldsymbol{M}=\boldsymbol{M}\cdot\boldsymbol{L}=0 \tag{4}$$

and

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

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

$$\boldsymbol{B}=(\mu/2E)^{1/2}\boldsymbol{M} \tag{6}$$

equations (4) and (5) specialise to

$$\boldsymbol{L}\cdot\boldsymbol{B}=\boldsymbol{B}\cdot\boldsymbol{L}=0 \tag{7}$$

and

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

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

$$[L_j, L_k]=\mathrm{i}\hbar\varepsilon_{jkl}L_l, \qquad [L_j, B_k]=\mathrm{i}\hbar\varepsilon_{jkl}B_l, \qquad [B_j, B_k]=-\mathrm{i}\hbar\varepsilon_{jkl}L_l. \tag{9}$$

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

$$\left.\begin{aligned} L_j&=\tfrac{1}{2}(a^+\sigma_j a+b^+\sigma_j b)\hbar\\ B_j&=\tfrac{1}{2}(a^+\sigma_j C\tilde{b}^+-\tilde{a}C\sigma_j b)\hbar\end{aligned}\right\}, \qquad j=1,2,3,$$
$$a=\begin{bmatrix}a_1\\a_2\end{bmatrix}, \qquad b=\begin{bmatrix}a_3\\a_4\end{bmatrix}, \qquad C=\begin{pmatrix}0&-1\\1&0\end{pmatrix}, \tag{10}$$

where σ_j ($j=1,2,3$) are the standard Pauli matrices and where a_j and a_j^+ ($j=1,2,3,4$) are annihilation and creation Bose operators. (In passing we note in view of preparing the result below concerning SO(4, 2) that the 36 possible bilinear forms of a_j and a_j^+ ($j=1,2,3,4$) span the Lie algebra of the symplectic group $\mathrm{Sp}(8, R)$.) Then, we introduce equations (10) into (7) and (8). As a result, equation (7) yields

$$(a_1^+a_1+a_2^+a_2-a_3^+a_3-a_4^+a_4)(a_1^+a_4^+ +a_1a_4-a_2^+a_3^+ -a_2a_3)=0 \tag{11}$$

and equation (8) leads to

$$(a_1^+a_1+a_2^+a_2-a_3^+a_3-a_4^+a_4)^2-(a_1^+a_4^+ +a_1a_4-a_2^+a_3^+ -a_2a_3)^2=-2\mu(Ze^2)^2/(E\hbar^2). \tag{12}$$

(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 bosonised expressions (11) and (12) can be combined to give the solution

$$a_1^+a_1+a_2^+a_2-a_3^+a_3-a_4^+a_4=0 \tag{13}$$

and

$$(a_1^+a_4^+ +a_1a_4-a_2^+a_3^+ -a_2a_3)^2=2\mu(Ze^2)^2/(E\hbar^2). \tag{14}$$

We now show that equation (14) is amenable to a form that parallels that 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

$$Q_j=\tfrac{1}{2}(2\hbar/\mu\omega)^{1/2}(a_j+a_j^+), \qquad P_j=\tfrac{1}{2}(2\hbar\mu\omega)^{1/2}(a_j-a_j^+)/\mathrm{i}, \tag{15}$$

equation (14) reads

$$(2\mu)^{-1}P_1P_4-\tfrac{1}{2}\mu\omega^2Q_1Q_4-(2\mu)^{-1}P_2P_3+\tfrac{1}{2}\mu\omega^2Q_2Q_3=\omega(\mu/2E)^{1/2}Ze^2. \tag{16}$$

An evident canonical transformation $\{P_j, Q_j: j=1,2,3,4\}\rightarrow\{P_j', Q_j': j=1,2,3,4\}$

allows us to obtain finally

$$\frac{1}{2\mu}\sum_{j=1}^{4} P'^2_j - \tfrac{1}{2}\mu\omega^2 \sum_{j=1}^{4} Q'^2_j = \omega(2\mu/E)^{1/2}Ze^2, \tag{17}$$

to be compared with equation (2).

We thus end up with the result that the continuum states of an $\mathbb{R}^3$ hydrogen atom are connected with continuum states of an $\mathbb{R}^4$ isotropic harmonic oscillator with negative potential energy (cf equation (17)) accompanied by 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 1983). 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 an $\mathbb{R}^4$ 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 1983) 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 $\mathrm{Sp}(8, R)$ spanned by the set $\{a_j^+a_k^+, a_j^+a_k, a_ja_k : j \text{ and } k = 1, 2, 3, 4\}$ 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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