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On the q -analogue of the hydrogen atom

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Abstract. The discrete spectrum of a q -analogue of the hydrogen atom is obtained from a deformation of the Pauli equations. As an alternative, the spectrum is derived from a deformation of the four-dimensional oscillator arising in the application of the Kustaanheimo–Stiefel transformation to the hydrogen atom. A model of the 2s–2p Dirac shift is proposed in the context of q -deformations.

1. Introduction

In recent years, much work has been devoted to an apparently new mathematical structure, the structure of a quantum group, and its application to various fields of physics (statistical mechanics, conformal quantum field theory, etc). Indeed, the structure of a quantum group (or algebra) is connected with those of Hecke algebra and quasi-triangular Hopf algebra and certainly plays an important role in non-commutative geometry (Drinfel'd 1985, Jimbo 1985, Woronowicz 1987). Loosely speaking, the structure of a quantum algebra corresponds to a deformation which can be characterized by a deformation parameter q , an arbitrary complex number in the most general case.

There is no universal significance in the parameter q and the physicist is tempted to consider it as a phenomenological parameter, something like a curvature constant, to be adjusted to the experimental data. The limiting situation $q = 1$ corresponds to the flat case and gives back the results afforded by (ordinary) quantum mechanics. For example, when q goes to 1, the quantum algebra $su_q(2)$, which defines a q -analogue of angular momentum, reduces to the Lie algebra $su(2)$ of (ordinary) angular momentum. The algebra $su(2)$ is used from atoms to quarks with some reasonable success and, therefore, the replacement of $su(2)$ by $su_q(2)$ with q near to 1 should be appropriate for the description of fine structure effects. In the framework of this philosophy, we may expect to obtain a fine structure of the hydrogen atom from a deformation of its non-relativistic spectrum.

It seems interesting to investigate q -analogues of dynamical systems in view of their potential use as refined units for modelling physical systems, with the case $q \rightarrow 1 = 0$ corresponding to already known effects and the case $q - 1 \simeq 0$ to new effects (such as, for instance, spectrum shift and spectrum splitting). In this vein, the q -analogue of the harmonic oscillator, as derived among others by Macfarlane (1989), Biedenharn (1989), Sun and Fu (1989) and Kulish and Reshetikhin (1989), represents a first important

st.p; further, the q -analogues of various coherent states introduced recently (Quesne 1991, Katriel and Solomon 1991) might be interesting in physical applications.

It is the purpose of the present work to introduce a q -analogue of another very simple dynamical system, that is the three-dimensional hydrogen atom. We shall deal here with the (quantum mechanical) discrete spectrum of the hydrogen atom in \mathbb{R}^3 and shall obtain in section 2 its q -analogue by passing from the dynamical invariance algebra $\mathfrak{so}(4) = \mathfrak{su}(2) \oplus \mathfrak{su}(2)$ of the ordinary hydrogen atom system to its q -analogue $\mathfrak{su}_q(2) \oplus \mathfrak{su}_q(2)$. In section 3, an alternative spectrum will be derived from the Kustaanheimo-Stiefel (KS) transformation (Kustaanheimo and Stiefel 1965) and applied to a phenomenological derivation of the 2s-2p fine structure splitting. We shall close this article with some conclusions in section 4 about the non-unicity of q -analogues and the relevance of the quantum algebra $\mathfrak{so}_q(3, 2)$ for the Wigner-Racah algebra of $SU_q(2)$

2. q -analogue of the Pauli equations

Since we want to examine $\mathfrak{su}_q(2) \oplus \mathfrak{su}_q(2)$, we review, in a non-standard presentation, some basic facts about the quantum algebra $\mathfrak{su}_q(2)$. Let $\mathcal{E} = \{|jm\rangle : 2j \in \mathbb{N}, m = -j(1+j)\}$ be the Hilbert space of the representation theory of the (ordinary) Lie group $SU(2)$. We define the operators a_+ , a_+^\dagger , a_- and a_-^\dagger acting on \mathcal{E} by the relationships

$$\begin{aligned} a_\pm |jm\rangle &= \sqrt{[j \pm m]} |j - \frac{1}{2}, m \mp \frac{1}{2}\rangle \\ a_\pm^\dagger |jm\rangle &= \sqrt{[j \pm m + 1]} |j + \frac{1}{2}, m \pm \frac{1}{2}\rangle. \end{aligned} \quad (1)$$

In equation (1), we use the notation $[x] \equiv [x]_q$ where

$$[x]_q = \frac{q^x - q^{-x}}{q - q^{-1}} \quad (2)$$

is the q -analogue of the (real) number x ; q is taken as a complex number which is not a root of unity. In the limiting situation $q = 1$, equation (1) gives back the defining relationships introduced by Schwinger (1952) in his theory of angular momentum (see also Kibler and Grenet (1980) and Nomura (1990)). Some trivial properties (matrix elements, time-reversal behaviour, adjointness relationships, etc) for the operators a_+ , a_+^\dagger , a_- and a_-^\dagger can be derived from the initial relationship (1).

By introducing

$$n_1 = j + m \quad n_2 = j - m \quad |jm\rangle \equiv |j + m, j - m\rangle = |n_1, n_2\rangle \quad (3)$$

we immediately obtain

$$\begin{aligned} a_+ |n_1 n_2\rangle &= \sqrt{[n_1]} |n_1 - 1, n_2\rangle & a_+^\dagger |n_1 n_2\rangle &= \sqrt{[n_1 + 1]} |n_1 + 1, n_2\rangle \\ a_- |n_1 n_2\rangle &= \sqrt{[n_2]} |n_1, n_2 - 1\rangle & a_-^\dagger |n_1, n_2\rangle &= \sqrt{[n_2 + 1]} |n_1, n_2 + 1\rangle. \end{aligned} \quad (4)$$

Consequently, the sets $\{a_+, a_+^\dagger\}$ and $\{a_-, a_-^\dagger\}$ are two commuting sets of q -bosons. Indeed, these q -bosons satisfy the relationships

$$\begin{aligned} a_+ a_+^\dagger - q^{-1} a_+^\dagger a_+ &= q^{N_1} & a_- a_-^\dagger - q^{-1} a_-^\dagger a_- &= q^{N_2} \\ [a_+, a_-]_- &= [a_+^\dagger, a_-^\dagger]_- = [a_+, a_-^\dagger]_- = [a_+^\dagger, a_-]_- = 0 \end{aligned} \quad (5)$$

where N_1 and N_2 are the (usual) number operators defined by

$$N_1|n_1n_2\rangle = n_1|n_1n_2\rangle \quad N_2|n_1n_2\rangle = n_2|n_1n_2\rangle. \quad (6)$$

Equations (4)–(6) show that each of the sets $\{a_+, a_+^\dagger\}$ and $\{a_-, a_-^\dagger\}$ is a set of q -bosons as introduced independently by many authors including Macfarlane (1989), Biedenharn (1989) and Sun and Fu (1989).

We now introduce the following three operators

$$J_- = a_-^\dagger a_+ \quad J_3 = \frac{1}{2}(N_1 - N_2) \quad J_+ = a_+^\dagger a_-. \quad (7)$$

The action of J_- , J_3 and J_+ on the space \mathcal{E} is given by

$$J_3|jm\rangle = m|jm\rangle \quad J_\pm|jm\rangle = \sqrt{[j \mp m][j \pm m + 1]}|j, m \pm 1\rangle \quad (8)$$

We thus recover the Jimbo representation of the quantum group $SU_q(2)$. The commutation relationships of the operators J_- , J_3 and J_+ easily follow from (8). As a matter of fact, we have

$$[J_3, J_\pm]_- = \pm J_\pm \quad [J_+, J_-]_- = [2J_3]. \quad (9)$$

In equation (9), the abbreviation $[A] \equiv [A]_q$ stands for the q -analogue

$$[A]_q = \frac{q^A - q^{-A}}{q - q^{-1}} \quad (10)$$

of the operator A acting on \mathcal{E} . The relationships (9) characterize the quantum algebra $su_q(2)$.

A basic ingredient of $su_q(2)$, of central importance for what follows, is its Casimir operator J^2 . We shall take it in the form

$$J^2 = \frac{1}{2}(J_+ J_- + J_- J_+) + \frac{1}{2}[2][J_3]^2 \quad (11)$$

so that the eigenvalues of J^2 on \mathcal{E} are $[j][j + 1]$ with $2j$ in \mathbb{N} . The form taken here for J^2 differs from the one usually encountered in the literature; indeed, equation (11) ensures that the eigenvalues of J^2 are merely $j(j + 1)$ in the limiting case $q = 1$, a result which turns out to be essential in the framework of the philosophy sketched in the introduction.

We are in a position to q -deform the Pauli equations for the three-dimensional hydrogen atom in the case of the discrete spectrum. From the orbital angular momentum L and the Laplace–Runge–Lenz–Pauli vector M for the ordinary hydrogen atom system, we define the operators A and B through

$$A = \frac{1}{2}(L + N) \quad B = \frac{1}{2}(L - N) \quad N = \sqrt{\frac{-\mu}{2E}} M \quad (12)$$

where E is the energy ($E < 0$) and μ the reduced mass of the atom. We know that $\{A_i : i = 1, 2, 3\}$ and $\{B_i : i = 1, 2, 3\}$ are the generators of two groups, say $ASU(2)$

and $BSU(2)$, both of them being of the $SU(2)$ type. In addition, the Casimir operators A^2 and B^2 of the Lie algebras $asu(2)$ and $bsu(2)$ satisfy the equations (see Pauli 1926)

$$A^2 - B^2 = 0 \quad E(2A^2 + 2B^2 + \hbar^2) = -\frac{1}{2}\mu Z^2 e^4 \quad (13)$$

valid for a hydrogen-like atom with a nuclear charge Ze . A possible way to define a q -deformed hydrogen atom is to deform the Lie groups $ASU(2)$ and $BSU(2)$. Then, the Pauli equations (13) have to be extended to the quantum algebra $asu_q(2) \oplus bsu'_q(2)$. This deformation produces a q -analogue of the hydrogen atom, the energy \bar{E} of which is given by

$$E \equiv E_j = \frac{1}{4[j][j+1] + 1} E_0 \quad 2j \in \mathbb{N} \quad (14)$$

with

$$E_0 = -\frac{1}{2} \frac{\mu Z^2 e^4}{\hbar^2}. \quad (15)$$

Equations (14) and (15) follow from (13) where we have introduced the eigenvalues of A^2 and B^2 , in correct units, of the Casimir operators of $asu_q(2)$ and $bsu_q(2)$.

The quantity E_0 is the energy of the ground state of the q -deformed hydrogen atom. The q -deformed hydrogen atom defined by (14) thus has the same ground energy level as the ordinary hydrogen atom which corresponds to the limiting situation $q = 1$. Furthermore, its (discrete) spectrum exhibits the same degeneracy as that of the ordinary hydrogen atom. The only difference between the cases $q = 1$ and $q \neq 1$ arises in the position of the excited levels. Of course, the q -deformed spectrum reduces to that of the ordinary hydrogen atom when q goes to 1; the principal quantum number n is then given by $n = 2j + 1$.

3. q -analogue and KS transformation

In the case $q = 1$, we know how to pass from the hydrogen atom in \mathbb{R}^3 to an isotropic harmonic oscillator in \mathbb{R}^4 or $\mathbb{R}^2 \otimes \mathbb{R}^2$ by applying the KS transformation (Boiteux 1972, Kibler and Négadi 1983a, b, 1984, Kibler *et al* 1986). The reader may consult Kustaanheimo and Stiefel (1965), Cornish (1984), Lambert and Kibler (1988), and Hage Hassan and Kibler (1991) for a description of this transformation, which is indeed a particular Hurwitz transformation. The KS transformation can be used to define a q -deformed hydrogen atom. This may be achieved along the following lines: (i) apply the KS transformation to the ordinary hydrogen atom in \mathbb{R}^3 in order to obtain an isotropic harmonic oscillator in \mathbb{R}^4 ; (ii) transpose the latter oscillator into its q -analogue; and (iii) invoke the 'inverse' KS transformation to obtain a q -analogue of the hydrogen atom.

As a result, we obtain a q -deformed hydrogen atom characterized by the discrete spectrum

$$E \equiv E_{n_1 n_2 n_3 n_4} = \frac{16}{\nu(n_1 n_2 n_3 n_4)^2} E_0 \quad (16a)$$

$$\nu(n_1 n_2 n_3 n_4) = \sum_{i=1}^4 ([n_i] + [n_i + 1]) \quad n_i \in \mathbb{N} \quad (i = 1, 2, 3, 4). \quad (16b)$$

In the limiting case $q = 1$, the principal quantum number n is connected to the oscillator quantum numbers n_i ($i = 1, 2, 3, 4$) by $n_1 + n_2 + n_3 + n_4 + 2 = 2n$. Then, the q -deformed spectrum (16) gives back the discrete spectrum of the ordinary hydrogen atom when q goes to 1. Here again, the q -deformed hydrogen atom has the same ground energy level as the ordinary hydrogen atom. However, we now pass from the discrete spectrum of the ordinary hydrogen atom to the one of this alternative q -deformed hydrogen atom by means of a level splitting for the excited levels.

As an illustration, the level corresponding to the principal quantum number $n = 2$ when $q = 1$ is split into two levels when $q \neq 1$. In fact, we have the two energy levels

$$E_{2000} = \frac{16}{([2] + [3] + 3)^2} E_0 \quad E_{1100} = \frac{4}{([2] + 2)^2} E_0. \quad (17)$$

We thus have a splitting of the $n = 2$ non-relativistic level, a situation which is reminiscent of the fine structure splitting afforded by the Dirac theory of the hydrogen atom. By using the oscillator basis $\{\bar{\Phi}_{n_1 n_2 n_3 n_4}\}$ described by Kibler *et al* (1986), it can be proved that the wavefunctions Ψ_{nlm} corresponding to the limiting case $q = 1$ are

$$\begin{aligned} \Psi_{200} &= N(\bar{\Phi}_{2000} + \bar{\Phi}_{0200} + \bar{\Phi}_{0020} + \bar{\Phi}_{0002}) \\ \Psi_{210} &= N(\bar{\Phi}_{2000} + \bar{\Phi}_{0200} - \bar{\Phi}_{0020} - \bar{\Phi}_{0002}) \end{aligned} \quad (18)$$

for (the doublet) E_{2000} , and

$$\begin{aligned} \Psi_{211} &= N[\bar{\Phi}_{1010} - \bar{\Phi}_{0101} + i(\bar{\Phi}_{1001} - \bar{\Phi}_{0110})] \\ \Psi_{21-1} &= N[\bar{\Phi}_{1010} - \bar{\Phi}_{0101} - i(\bar{\Phi}_{1001} - \bar{\Phi}_{0110})] \end{aligned} \quad (19)$$

for (the doublet) E_{1100} . Equation (17) illustrates the fact that, when going from $q = 1$ to $q \neq 1$, the spectrum is not only shifted but also split (except for the ground energy level). From (17), we obtain the splitting

$$\Delta_q = E_{1100} - E_{2000} = \frac{3}{16} E_0 (q - 1)^2 \quad \text{for } q - 1 \simeq 0. \quad (20)$$

We note that by taking $q = 1.004$, we get $\Delta_q = 0.33 \text{ cm}^{-1}$. The value obtained for Δ_q has the order of magnitude of the $(2p^{-2}P_{3/2}) - (2s^2S_{1/2}, 2p^2P_{1/2})$ experimental fine structure splitting.

4. Closing remarks

The application of quantum groups to a large class of physical problems requires the q -deformation of the usual dynamical systems. In this direction, the q -deformation of the one-dimensional harmonic oscillator (Macfarlane 1989, Biedenharn 1989) has been a decisive step. The q -analogues of the hydrogen atom in \mathbb{R}^3 introduced in this work represent a further important step. Part of this work might be extended to the hydrogen atom in \mathbb{R}^5 by means of the Hurwitz transformation associated with the Hopf fibration on spheres $S^7 \rightarrow S^4$ of compact fibre S^3 (Lambert and Kibler 1988, Hage Hassan and Kibler 1991).

The hydrogen atom in \mathbb{R}^3 is a basic dynamical system in classical and quantum mechanics in the case $q = 1$. (Ordinary quantum mechanics can be thought to correspond to the limiting case $q = 1$.) This system is maximally super-integrable (Evans 1990, Kibler and Winternitz 1990) with rich dynamical invariance and non-invariance algebras. It would be interesting to investigate invariance and non-invariance algebras of the q -deformed hydrogen atom and to see the branching rules when going from $q = 1$ (ordinary quantum mechanics) to $q \neq 1$ (q -deformed quantum mechanics). Similar remarks apply to the isotropic harmonic oscillator in \mathbb{R}^3 , another maximally super-integrable system.

There are several ways to define a q -analogue of the hydrogen atom. We have been concerned in this article with two of them. There are other solutions connected with pairs of non-commuting q -bosons. The two q -deformed hydrogen atoms defined in sections 3 and 4 by their discrete spectra are different although having the same (ordinary) quantum limit (corresponding to $q = 1$). This constitutes in fact a general problem we face when dealing with q -deformed objects (cf, for example, the case of coherent states introduced by Katriel and Solomon (1991)). We currently do not have a simple correspondence principle for associating a (unique) q -analogue to a given mathematical or physical object. The use of a clearly defined, via the notion of a q -derivative, q -deformed Schrödinger equation should lead to some standardization of q -deformed objects.

Among the two q -deformed hydrogen atoms discussed previously, the one obtained via the KS transformation is certainly the most interesting. It leads to a spectrum which is shifted and split with respect to the ordinary quantum limit corresponding to $q = 1$. Furthermore, the $2s-2p$ Dirac splitting can be reproduced by adjusting the value of q and this yields a value close to 1. The latter result should not be taken too seriously but it constitutes a model of the $2s - 2p$ splitting without relativistic quantum mechanics.

We close this section with a remark about the q -bosonization (7) of the spherical angular momentum $\{J_-, J_3, J_+\}$ leading to $su_q(2)$. We may also define an hyperbolic angular momentum $\{K_-, K_3, K_+\}$ by

$$K_- = a_+ a_- \quad K_3 = \frac{1}{2}(N_1 + N_2 + 1) \quad K_+ = a_+^\dagger a_-^\dagger \quad (21)$$

with the property

$$\begin{aligned} K_- |jm\rangle &= \sqrt{[j-m][j+m]} |j-1, m\rangle \\ K_3 |jm\rangle &= (j + \frac{1}{2}) |jm\rangle \\ K_+ |jm\rangle &= \sqrt{[j-m+1][j+m+1]} |j+1, m\rangle. \end{aligned} \quad (22)$$

The operators K_- , K_3 and K_+ satisfy the commutation relationships

$$[K_3, K_\pm]_- = \pm K_\pm \quad [K_+, K_-]_- = -[2K_3] \quad (23)$$

and thus span the quantum algebra $su_q(1, 1)$. There are four other bilinear forms of the q -bosons a_+ , a_+^\dagger , a_- and a_-^\dagger which can be formed in addition to the J s and the K s, as follows

$$k_+^\dagger = -a_+^\dagger a_+^\dagger \quad k_-^\dagger = a_-^\dagger a_-^\dagger \quad k_-^- = -a_+ a_+ \quad k_+^- = a_- a_- \quad (24)$$

The operators k_s are clearly shift operators for the quantum numbers j and m . It can be proved that the set $\{k_+^+, k_+^-, k_-^-, k_-^+\}$ span, together with the sets $\{J_-, J_3, J_+\}$ and $\{K_-, K_3, K_+\}$, a quantum algebra which may be identified to $so(3, 2) \simeq sp(4, \mathbb{R})$ when q goes to 1. The quantum algebra $so_q(3, 2)$ might be useful for studying the Wigner-Racah algebra of the group $SU_q(2)$ as was done in the case $q = 1$ (Kibler and Grenet 1980).

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