MISCELLANEOUS PHYSICAL APPLICATIONS
OF QUANTUM ALGEBRAS*

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Abstract

Some ideas about phenomenological applications of quantum algebras to physics are reviewed. We examine in particular some applications of the algebras $U_q(su_2)$ and $U_{qp}(u_2)$ to various dynamical systems and to atomic and nuclear spectroscopy. The lack of a true (unique) $q$- or $qp$-quantization process is emphasized.

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Abstract

Some ideas about phenomenological applications of quantum algebras to physics are reviewed. We examine in particular some applications of the algebras $U_q(su_2)$ and $U_{qp}(u_2)$ to various dynamical systems and to atomic and nuclear spectroscopy. The lack of a true (unique) q- or qp-quantization process is emphasized.

1. Introduction

The concept of quantized universal enveloping algebras (or quantum algebras) introduced in the eighties continues to be the object of numerous developments in mathematics and physics. Quantum algebras may be realized in terms of $q$-deformed bosons. The various physical applications of $q$-bosons and quantum algebras may be naively classified in four types.

1. In a problem involving ordinary bosons or ordinary harmonic oscillators or ordinary angular momenta (orbital, spin, isospin, · · · angular momenta) or, more generally, any ordinary dynamical system, one may think of replacing them by their $q$-analogues. If the limiting case where $q = 1$ describes the problem in a reasonable way, one may expect that the case where $q$ is close to 1 can describe some fine structure effects. In this approach, the (dimensionless) parameter $q$ is a further fitting parameter describing additional degrees of freedom; the question in this
approach is to find a physical interpretation of the (fine structure or anisotropy or curvature) parameter $q$. Along this first type, we have the following applications.

(i) Use of $q$-deformed oscillators for describing the interaction between matter and radiation.

(ii) Use of $q$-deformed oscillators and application of the quantum algebra $U_q(su_{1,1})$ to vibrational spectroscopy of molecules.

(iii) Application of the quantum algebra $U_q(su_{2})$, and even $U_q(u_2)$, to vibrational-rotational spectroscopy of molecules and nuclei.

Note that, in connection with these utilizations and applications, we may ask whether $q$-bosons should obey some $q$-deformed Bose-Einstein statistics.

2. A second type of applications concerns the more general situation where a physical problem is well described by a given (simple) Lie algebra $g$. One may then consider to associate a quantized universal enveloping algebra $U_q(g)$ to the Lie algebra $g$. Symmetries described by the Lie algebra $g$ are thus replaced by symmetries inherent to the quantum algebra $U_q(g)$. For generic $q$ (excluding the case where $q$ is a root of unity), the representation theory of $U_q(g)$ is connected to the one of $g$ in a trivial manner since any irreducible representation of $g$ provides us with an irreducible representation of $U_q(g)$. Here again, the case where $q$ is close to 1 may serve to describe fine structure effects.

3. A third type arises by allowing the deformation parameter $q$ not to be restricted to (real or complex) values close to 1. Completely unexpected results may result from this approach. This is the case for instance when $q$ is a root of unity for which case the representation theory of the quantum algebra $U_q(g)$ may be very different from the one of $g$. This may be also the case when $q$ takes values (in $\mathbb{R}$ or in $S^1$) far from unity.

4. Finally, a fourth type concerns more fundamental applications (more fundamental in the sense that the deformation parameter $q$ is not subjected to fitting procedures). We may mention, among others, applications to statistical mechanics, gauge theories, conformal field theories and so on. Also, quantum algebras might be interesting for a true definition of the quantum space-time.

We shall deal here with physical applications (mainly of a phenomenological nature) of type 1 to 3. We shall give a survey of ideas around some prototypical applications of quantum algebras corresponding to deformations of the Lie algebra $g = A_1$. Most of the applications have been concerned up to now with only one parameter (say $q$). The introduction of a second parameter (say $p$) should permit more flexibility. Therefore, we shall briefly discuss in section 2 a particular
version of a two-parameter quantum algebra $U_{qp}(u_2)$. Then, we shall consider applications to: (i) some nonrelativistic dynamical systems, with an emphasis on the Coulomb system which plays a so important role in atomic spectroscopy and quantum chemistry (section 3), (ii) the classification of chemical elements (section 4), and (iii) rotational spectroscopy of molecules and atomic nuclei (section 5). We shall limit ourselves in sections 2-5 to some results with a minimal bibliography. (Further references can be obtained from the quoted literature.) Some conclusions shall be given in section 6.

The author thanks the organizers of the symposium on "Generalized Symmetries in Physics" for inviting him to give this lecture.

2. The quantum algebra $U_{qp}(u_2)$

The quantum algebra $U_{qp}(u_2)$ can be easily introduced in the oscillator representation [1]. Let us start by defining the linear operators $a_+, a_+, a_-, a_-$ by the relations

$$a_+ |n_1 \rangle \otimes |n_2 \rangle = \sqrt{[[n_1 + \frac{1}{2} - \frac{1}{2}]]_{qp} |n_1 - 1 \rangle \otimes |n_2 \rangle}$$

$$a_+^+ |n_1 \rangle \otimes |n_2 \rangle = \sqrt{[[n_1 + \frac{1}{2} + \frac{1}{2}]]_{qp} |n_1 + 1 \rangle \otimes |n_2 \rangle}$$

$$a_- |n_1 \rangle \otimes |n_2 \rangle = \sqrt{[[n_2 + \frac{1}{2} - \frac{1}{2}]]_{qp} |n_1 \rangle \otimes |n_2 - 1 \rangle}$$

$$a_-^+ |n_1 \rangle \otimes |n_2 \rangle = \sqrt{[[n_2 + \frac{1}{2} + \frac{1}{2}]]_{qp} |n_1 \rangle \otimes |n_2 + 1 \rangle}$$

(with $a_+ |0 \rangle \otimes |0 \rangle = a_- |0 \rangle \otimes |0 \rangle = 0$), where $|n_1 n_2 \rangle$ is an (undeformed) vector defined on a two-particle Fock space $F_1 \otimes F_2$. In this paper, we use the notations

$$[[X]]_{qp} = \frac{q^X - p^X}{q - p} \quad [X]_q \equiv [[X]]_{qq^{-1}} = \frac{q^X - q^{-X}}{q - q^{-1}}$$

where $X$ may stand for an operator or a number. The sets $\{a_+, a_+^+\}$ and $\{a_-, a_-^+\}$ are two commuting sets of $qp$-bosons. More precisely, from (1) we have

$$a_+ a_+^+ - p a_+^+ a_+ = q^{N_1} \quad a_+ a_+^+ - q a_+^+ a_+ = p^{N_1}$$

$$a_- a_-^+ - p a_-^+ a_- = q^{N_2} \quad a_- a_-^+ - q a_-^+ a_- = p^{N_2}$$

$$[a_+, a_-] = [a_+, a_] = [a_+, a_-^+] = [a_+, a_-^-] = 0$$

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where the number operators $N_1$ and $N_2$ are defined via

$$N_i|n_1\rangle \otimes |n_2\rangle = n_i|n_1\rangle \otimes |n_2\rangle \quad (i = 1, 2) \quad (4)$$

as in the nondeformed case.

By introducing

$$n_1 = j + m \quad n_2 = j - m \quad n_1 \in \mathbb{N} \quad n_2 \in \mathbb{N} \quad (5a)$$

and

$$|jm\rangle \equiv |j + m, j - m\rangle = |n_1\rangle \otimes |n_2\rangle \in \mathcal{F}_1 \otimes \mathcal{F}_2 \quad (5b)$$

equation (1) can be rewritten in the form

$$a_+ |jm\rangle = \sqrt{[[j + m + \frac{1}{2} - \frac{1}{2}]_q]_p} |j - \frac{1}{2} m - \frac{1}{2}\rangle$$

$$a_+^+ |jm\rangle = \sqrt{[[j + m + \frac{1}{2} + \frac{1}{2}]_q]_p} |j + \frac{1}{2} m + \frac{1}{2}\rangle$$

$$a_- |jm\rangle = \sqrt{[[j - m + \frac{1}{2} - \frac{1}{2}]_q]_p} |j - \frac{1}{2} m + \frac{1}{2}\rangle$$

$$a_-^+ |jm\rangle = \sqrt{[[j - m + \frac{1}{2} + \frac{1}{2}]_q]_p} |j + \frac{1}{2} m - \frac{1}{2}\rangle$$

(6)

From equation (6), we see that we can construct bilinear forms of the operators $a_+$, $a_+^+$, $a_-$, and $a_-^+$ which behave like step operators on the $j$'s and/or $m$'s. Indeed, the ($qp$-deformed spherical angular momentum) operators

$$J_- = a_+^+ a_+ \quad J_3 = \frac{1}{2} (N_1 - N_2) \quad J_0 = \frac{1}{2} (N_1 + N_2) \quad J_+ = a_+^+ a_- \quad (7)$$
satisfy

$$J_- |jm\rangle = \sqrt{[[j + m]_q]_p} [ [j - m + 1]_q]_p |j, m - 1\rangle$$

$$J_3 |jm\rangle = m |jm\rangle \quad J_0 |jm\rangle = j |jm\rangle$$

$$J_+ |jm\rangle = \sqrt{[[j - m]_q]_p} [ [j + m + 1]_q]_p |j, m + 1\rangle$$

(8)

Hence, the commutators of the operators $J_-$, $J_3$, $J_0$, and $J_+$ are

$$[J_0, J_{\alpha}] = 0 \quad [J_3, J_{\pm}] = \pm J_{\pm} \quad [J_+, J_-] = (qp)^{J_0 - J_3} [ [2J_3]_q]_p \quad (9)$$

where $\alpha = -, 3, +$.  

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In a similar way, the \((qp\text{-deformed hyperbolic angular momentum})\) operators

\[
K_- = a_+ a_- \quad K_3 = \frac{1}{2} (N_1 + N_2 + 1) \equiv J_0 + \frac{1}{2} \quad K_+ = a_+^\dagger a_-^\dagger
\]  

(10)
satisfy

\[
K_- |jm\rangle = \sqrt{[j - m + 1 - \frac{1}{2}]_q [j + m + 1 - \frac{1}{2}]_q} |j-1,m\rangle
\]

\[
K_3 |jm\rangle = (j + \frac{1}{2}) |jm\rangle
\]

\[
K_+ |jm\rangle = \sqrt{[j - m + 1 + \frac{1}{2}]_q [j + m + 1 + \frac{1}{2}]_q} |j+1,m\rangle
\]

(11)
The commutators of the operators \(K_-, K_3, J_3, \) and \(K_+\) are

\[
[J_3, K_\alpha] = 0 \quad [K_3, K_\pm] = \pm K_\pm
\]

\[
[K_+, K_-] = -[[2K_3]]_q + (1 - qp)[[K_3 + J_3 - \frac{1}{2}]]_q[[K_3 - J_3 - \frac{1}{2}]]_q
\]

(12)
from which we recognize the Lie brackets of \(u_{1,1}\) when \(q = p^{-1} \rightarrow 1\).

Equations (9) and (12) are the starting point for generating the quantum algebras (as Hopf algebras) \(U_{qp}(u_2)\) and \(U_{qp}(u_{1,1})\), respectively. Note that we can form other bilinears, in the \(qp\)-boson operators, in addition to (7) and (10) ; this leads to the quantum algebra \(U_{qp}(o_{3,2})\) which is of special relevance for studying the “Wigner-Racah” algebras of \(U_{qp}(u_2)\) and \(U_{qp}(u_{1,1})\) [2,3]. We shall focus here on the algebra \(U_{qp}(u_2)\). For the applications, it is enough to mention that the co-product \(\Delta_{qp}\) of \(U_{qp}(u_2)\) is defined by

\[
\Delta_{qp}(J_\pm) = J_\pm \otimes (qp)^{\frac{1}{2} J_0 (qp^{-1}) + \frac{1}{2} J_3} + (qp)^{\frac{1}{2} J_0 (qp^{-1}) - \frac{1}{2} J_3} \otimes J_\pm
\]

\[
\Delta_{qp}(J_3) = J_3 \otimes I + I \otimes J_3 \quad \Delta_{qp}(J_0) = J_0 \otimes I + I \otimes J_0
\]

(13)
and that the operator

\[
C_2(U_{qp}(u_2)) = \frac{1}{2} (J_+ J_- + J_- J_+) + \frac{1}{2} [[2]]_q (qp)^{J_0 - J_3} [[J_3]]_q^2
\]

(14)
is an invariant of \(U_{qp}(u_2)\). The eigenvalue of the Casimir \(C_2(U_{qp}(u_2))\) on the subspace \(\{|jm\rangle : m = -j, -j + 1, \ldots, j\}\) is simply \([[j]]_q[[j + 1]]_q\). The quantum algebra \(U_{qp}(u_2)\) is a two-parameter quantum algebra. Note that the hermitean conjugation property \(J_\dagger = J_+\) requires that either \(q\) and \(p\) are real or \(p = \bar{q}\). The algebra \(U_{qp}(u_2)\) clearly leads to the “classical” quantum algebra \(U_q(su_2)\) when \(p = q^{-1}\) and \(U_q(su_2)\) yields in turn the Lie algebra \(su_2\) when \(q \rightarrow 1\).
We may wonder whether we really gain something when passing from the “classical” quantum algebra $U_q(su_2)$ to the quantum algebra $U_{qp}(u_2)$. In this connection, let us define the operators $A_{\alpha}$ ($\alpha = -, 3, 0, +$) through

$$J_{\pm} = (qp)^{\frac{1}{2}(A_0-\frac{1}{2})} A_{\pm} \quad J_0 = A_0 \quad J_3 = A_3$$

(15)

and let us introduce

$$Q = (qp^{-1})^{\frac{1}{2}} \quad P = (qp)^{\frac{1}{2}}$$

(16)

Then, we can verify that the set $\{A_-, A_3, A_+\}$ spans $U_Q(su_2)$, which commutes with $A_0$, so that we have central extension

$$U_{qp}(u_2) = u_1 \otimes U_Q(su_2)$$

(17)

On the other hand, the invariant $C_2(U_{qp}(u_2))$ can be developed as

$$C_2(U_{qp}(u_2)) = P^{2A_0-1} C_2(U_Q(su_2))$$

(18)

where

$$C_2(U_Q(su_2)) = \frac{1}{2} (A_+ A_- + A_- A_+) + \frac{1}{2} [2]_Q [A_3]_Q^2$$

(19)

is an invariant of $U_Q(su_2)$. Therefore, in spite of the fact that the transformation (15-16) allows us to generate the one-parameter algebra $U_Q(su_2)$ from the two-parameter algebra $U_{qp}(u_2)$, the invariant $C_2(U_{qp}(u_2))$ given by (18) still exhibits two independent parameters ($Q$ and $P$). For physical applications, the introduction of a second parameter gives more flexibility in fitting procedures and/or phenomenological approaches.

To close this section, it should be mentioned that multi-parameter (in particular two-parameter) quantum algebras have been studied by many authors (see for example Refs. [4-7]).

3. Application to dynamical systems

An important preliminary step for applying $q$-quantization processes is to know $q$- and/or $qp$-analogues of ordinary dynamical systems. We shall be interested here in nonrelativistic dynamical systems corresponding to a charged particle (of reduced mass $\mu = 1$) embedded in a scalar potential $V$. The case of a 4-potential, involving a vector potential (corresponding to an Aharonov-Bohm situation, or a monopole or a dyonium), can be addressed in a similar way.
Among the various dynamical systems used in physics, the oscillator system in \( \mathbb{R} \) and the Coulomb system in \( \mathbb{R}^3 \) are two paradigms of considerable importance. We shall briefly discuss \( qp \)-analogues for the latter two systems and for three parent systems [viz., the Smorodinsky-Winternitz (SW) system, the generalized oscillator system and the generalized Coulomb system]. In the following, we use units such that \( \hbar = 1 \).

1. The oscillator system. The oscillator system in \( \mathbb{R}^N \) is a superposition of one-dimensional oscillator systems corresponding to potentials of type \( V = \frac{1}{2} \Omega^2 x^2 \) with \( \Omega > 0 \). Such a system is maximally superintegrable with \( 2N - 1 \) constants of motion. For \( N = 1 \), the \( qp \)-quantization of the oscillator system may be achieved by extending (to \( p \neq q^{-1} \)) the recipe given independently by many authors (see Refs. [8-13]). The energy spectrum for the one-dimensional \( qp \)-deformed oscillator so-obtained reads

\[
E = \frac{1}{2} \Omega \left( [n]_{qp} + [n + 1]_{qp} \right) \quad n \in \mathbb{N}
\]

(20)

Note that \( E \) is real if \( q \) and \( p \) are real or if \( p = \bar{q} \). By using equation (16), formula (20) can be rewritten as

\[
E = \frac{1}{2} \Omega P^n \left( \frac{1}{P} [n]_Q + [n + 1]_Q \right)
\]

(21)

Two particular cases are of special interest when \( Q = q \) and \( P = 1 \) : For \( p^{-1} = q = e^{\psi} \) (with \( \psi \in \mathbb{R} \)), we have

\[
E = \frac{1}{2} \Omega \frac{\sinh(2n + 1)\psi}{\sinh \frac{\psi}{2}}
\]

(22)

while for \( p^{-1} = q = e^{i\varphi} \) (with \( \varphi \in \mathbb{R} \)), we obtain

\[
E = \frac{1}{2} \Omega \frac{\sin(2n + 1)\varphi}{\sin \frac{\varphi}{2}}
\]

(23)

The energy \( E \) as given by (22) or (23) can be expanded in terms of the nondeformed eigenvalue \( (\Omega/2)(n + 1/2) \).

2. The Coulomb system. The attractif Coulomb system in \( \mathbb{R}^3 \) corresponds to the potential \( V = \alpha(1/r) \) with \( \alpha < 0 \). This system is maximally superintegrable with five constants of motion. By applying the Kustaanheimo-Stiefel transformation (i.e., the Hopf fibration \( S^3 \to \mathbb{S}^2 \) of compact fiber \( S \)), we can transform the \( \mathbb{R}^3 \)}
Coulomb system into a coupled pair of $\mathbb{R}^2$ oscillator systems. The $qp$-quantization of the Coulomb system may thus be accomplished by $qp$-quantizing the $\mathbb{R}^2$ oscillator systems [14]. We thus obtain a $qp$-analogue of the Coulomb system in $\mathbb{R}^3$ for which the discrete energy spectrum is

$$E = \frac{1}{\nu^2} E_0 \quad E_0 = -\frac{1}{2} \alpha^2 \quad \nu = \frac{1}{4} \sum_{i=1}^{4} ([n_i]_{qp} + [n_i + 1]_{qp})$$

(24)

It should be noticed that a similar $qp$-quantization process can be effectuated for the Coulomb system in $\mathbb{R}^5$ by using the Hopf fibration $S^7 \to S^4$ of compact fiber $S^3$.

3. The Smorodinsky-Winternitz system. The SW system in $\mathbb{R}^N$ may be considered as a superposition of one-dimensional systems corresponding to potentials of type

$$V = \frac{1}{2} \Omega^2 x^2 + \frac{1}{2} P \frac{1}{x^2}$$

(25)

where $\Omega > 0$ and $P > 0$. The SW system was originally introduced for $N = 2$ [15]. For $N = 3$, the SW potential is of the $V_1$ type in the classification of Ref. [16]; this potential allows the separation of variables in the Schrödinger equation in eight systems of coordinates [17]. For $N$ arbitrary, the SW system is maximally superintegrable with $2N - 1$ constants of motion [17]. Going back to $N = 1$, we may $qp$-quantize the SW system by using the approach developed in [18,19]. The energy spectrum for the $qp$-deformed SW system so-obtained is discrete only and given by

$$E = \Omega \left( [n]_{qp} + [n + 1]_{qp} + \sqrt{\frac{1}{4} + P} \right) \quad n \in \mathbb{N}$$

(26)

In the case where $p^{-1} = q \to 1$, the energy $E$ reduces to the one for the nondeformed one-dimensional SW system [15,19] (note the sign in front of the square root, cf. Refs. [17,20]). It should be observed that, in the limiting situation for which $p^{-1} = q = 1$ and $P = 0$, corresponding to the ordinary oscillator system, we must replace (26) by $E = \Omega (n + n + 1 \pm \frac{1}{2}) = \Omega (k + \frac{1}{2})$ where $k$ may be equal to $2n + 1$ or $2n$.

4. The generalized oscillator system. This system corresponds in $\mathbb{R}^3$ to the potential [in circular cylindrical coordinates $(\rho, \varphi, z)$]

$$V = \frac{1}{2} \Omega^2 (\rho^2 + z^2) + \frac{1}{2} P \frac{1}{z^2} + \frac{1}{2} Q \frac{1}{\rho^2}$$

(27)
where $\Omega > 0$, $P > 0$, and $Q > 0$. The potential (27) is of the $V_3$ type in the classification of Ref. [16]. It allows the separation of variables in the Schrödinger equation in four systems of coordinates (spherical, circular cylindrical, prolate spheroidal, and oblate spheroidal coordinates). The three-dimensional generalized oscillator system is minimally superintegrable with four constants of motion. By using the approach of Ref. [19], we can derive a $qp$-analogue for this system. Its energy spectrum is given by

$$E = 2\Omega \nu \quad \nu = \frac{1}{2} \sum_{i=1}^{2} (\lfloor n_i \rfloor_{qp} + \lfloor n_i + 1 \rfloor_{qp} + |S_i|)$$

$$|S_1| = \sqrt{m^2 + Q} \quad |S_2| = \sqrt{\frac{1}{4} + P}$$

$$n_1 \in \mathbb{N} \quad n_2 \in \mathbb{N} \quad m \in \mathbb{Z}$$

and is discrete only.

5. The generalized Coulomb system. This system corresponds in $\mathbb{R}^3$ to the potential [in spherical coordinates $(r, \theta, \varphi)$]

$$V = \alpha \frac{1}{r} + \beta \frac{\cos \theta}{r^2 \sin^2 \theta} + \gamma \frac{1}{r^2 \sin^2 \theta}$$

(29)

where $\alpha < 0$ and $\gamma \geq |\beta|$. The potential (29) is of the $V_4$ type in the classification of Ref. [16]. It allows the separation of variables in the Schrödinger equation in spherical and parabolic coordinates. The three-dimensional generalized Coulomb system is minimally superintegrable with four constants of motion. By using the approach of Ref. [18], we can derive a $qp$-analogue for this system. Its discrete energy spectrum is

$$E = \frac{1}{\nu^2} E_0 \quad E_0 = -\frac{1}{2} \alpha^2 \quad \nu = \frac{1}{2} \sum_{i=1}^{2} (\lfloor n_i \rfloor_{qp} + \lfloor n_i + 1 \rfloor_{qp} + |S_i|)$$

$$|S_i| = \sqrt{m^2 + 2[\gamma + (-1)^i \beta]}$$

$$n_1 \in \mathbb{N} \quad n_2 \in \mathbb{N} \quad m \in \mathbb{Z}$$

(30)

Note that the occurrence of a similar quantum number $\nu$ in (28) and (30) is reminiscent of the well-known connection between harmonic oscillator system and Coulomb system.

For each of the $qp$-deformed systems 1 to 5, in the limiting situation for which $p^{-1} = q = 1$, we recover the spectra corresponding to the nondeformed systems. The case where $q$ and $p$ are close to 1 may be used for mimicking some perturbation effects. In this respect, let us consider the example of the hydrogen atom and of its
$q$-analogue (we take $p^{-1} = q$). We know that the level for the principal quantum number $n = 2$ (i.e., $\ell = 0$ and $\ell = 1$) exhibits a fourfold (or eightfold, if spin is taken into account) degeneracy corresponding to the subspace $2s(\ell = 0) \oplus 2p(\ell = 1)$. In the $q$-quantization picture, it can be shown from (24) that the $n = 2$ level splits into two doublets (or quartets, if spin is taken into account). Furthermore, the obtained level splitting exactly reproduces the Dirac splitting of the $n = 2$ level, namely, $(2p^2P_\frac{3}{2}) - (2s^2S_\frac{1}{2}, 2p^2P_\frac{1}{2})$, when

$$q = 1 + \frac{1}{\sqrt{3}} \alpha$$

(31)

where $\alpha$ stands here for the fine structure constant. We have here an application of type 1-2.

4. Application to chemical elements

Let us go now to an application of type 2-3. Atoms and ions can be builded from the filling, with some prescription (taking into account the Pauli exclusion principle), of the various $n\ell$ shells of the hydrogen atom. Neutral atoms are reasonably well-described by the ordering

$$1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p < 5s < 4d < 5p < 6s < 4f < 5d < 6p < 7s < 5f < 6d < \cdots$$

(32)

while positive monatomic ions correspond to the sequence

$$1s < 2s < 2p < 3s < 3p < 3d < 4s < 4p < 4d < 5s < 5p < 4f < 5d < 6s < 6p < 5f < 6d < 7s < \cdots$$

(33)

The filling of the atomic shells is thus different for atoms and ions. For instance, for the neutral atom Ti(I) we have the atomic configuration $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^2$ and for the tripositive ion Ti(IV) the filling is $1s^2 2s^2 2p^6 3s^2 3p^6 3d^1$.

We want to describe here an Aufbau Prinzip based on: (i) the use of the $\mathfrak{so}_4$ symmetry of the hydrogen atom, (ii) the breaking of the $\mathfrak{so}_4$ symmetry via an $\mathfrak{so}_3$ invariant term, (iii) the replacement of the chain $\mathfrak{so}_4 \supset \mathfrak{so}_3$ by the chain $\mathfrak{so}_4 > U_q(\mathfrak{so}_3)$, and (iv) the filling of the $n\ell$ shells arising from $\mathfrak{so}_4 > U_q(\mathfrak{so}_3)$ according to the Pauli principle.

Let us first briefly describe how the chain $\mathfrak{so}_4 \supset \mathfrak{so}_3$ occurs in this problem. By using the Fock stereographic projection, we know how to express the Hamiltonian
$H$ of the hydrogen atom as a function of the Hamiltonian $\Lambda^2$ [the eigenvalues of which are $\lambda(\lambda + 2)$ with $\lambda \in \mathbb{N}$] for the four-dimensional symmetric rotor. In convenient units, the operator $H$ reads

$$H = -\frac{1}{2} \frac{1}{\Lambda^2 + 1} \tag{34}$$

whose eigenvalues are $-(1/2)(1/n^2)$, where $n = \lambda + 1$ is the principal quantum number. Following Novaro [21], we may think to break the $so_4$ symmetry by replacing $\Lambda^2$ by $\Lambda^2 + \alpha L^2$, where the asymmetry parameter $\alpha$ is real and $L^2$ is the Casimir operator of $so_3$ [the eigenvalues of which are $\ell(\ell + 1)$ with $\ell \in \mathbb{N}$].

The replacement of the symmetric rotor by an asymmetric one thus introduces the orbital quantum number $\ell$. Then, the energy of the $n\ell$ shell is

$$E = -\frac{1}{2} \frac{1}{n^2 + \alpha \ell(\ell + 1)} \tag{35}$$

It is known that $\alpha = 4/3$ reproduces in a reasonable way the ordering (32) for neutral atoms [21]. However, there exists no value of $\alpha$ for reproducing in an acceptable way the ordering (33) for positive ions.

The next step is to $q$-quantize the chain $so_4 \supset so_3$. The minimal extension of the Novaro model is obtained by substituting the quantum algebra $U_q(so_3)$ to the Lie algebra $so_3$ [22]. This leads to a new Hamiltonian whose eigenvalues are given by (35) with the substitutions $\ell(\ell+1) \mapsto [\ell]_q[\ell+1]_q$ and $\alpha \mapsto \alpha(q)$. The dependence in $q$ is introduced not only at the level of the Casimir operator of $U_q(so_3)$ but also in the parameter $\alpha$. A simple model is obtained for $\alpha = 3 - (5/3)q$ which gives back $\alpha = 4/3$ for $q = 1$. The ordering of the $n\ell$ shells is thus controlled by the expression

$$n^2 + (3 - \frac{5}{3}q) [\ell]_q [\ell + 1]_q \tag{36}$$

From the latter expression, we obtain a good classification of: (i) neutral atoms for $q = 0.9$, (ii) positive monoatomic ions for $1.1 < q < 1.4$, and (iii) hydrogen-like ions for $1.4 < q < 1.8$. Note that the hydrogen atom corresponds to the limiting value $q = 9/5$. It is to be emphasized that the so-obtained classification of atoms is better than the one afforded by the Novaro model (that corresponds to $q = 1$).

5. Application to rotational spectroscopy

As a third application (indeed, an application of type 2), we now describe a model for rotational spectroscopy of molecules and nuclei. This model is based
upon the Hamiltonian
\[ H = \frac{1}{2\mathcal{I}} C_2(U_{qp}(u_2)) + E_0 \] (37)
where \( E_0 \) is some constant (e.g., the bandhead energy for a deformed or superdeformed nucleus) and \( \mathcal{I} \) denotes the moment of inertia of the nucleus or molecule under study. The diagonalization of \( H \) within a subspace of constant angular momentum \( J \) (a spin angular momentum for a nucleus or a molecular angular momentum for a molecule) leads to the energies
\[ E = \frac{1}{2\mathcal{I}} [[J]_{qp} [[J + 1]_{qp} + E_0 \] (38)
or equivalently
\[ E = \frac{1}{2\mathcal{I}} e^{(2J-1)\frac{s+r}{2}} \frac{\sinh(J\frac{s-r}{2}) \sinh[(J + 1)\frac{s-r}{2}]}{\sinh^2(\frac{s-r}{2})} + E_0 \] (39)
where we have introduced \( s = \ln q \) and \( r = \ln p \). For evident reasons, \( E \) should be real. Therefore, we can take either \( (s - r) \in \mathbb{R} \) and \( (s + r) \in \mathbb{R} \) or \( (s - r) \in \mathbb{i\mathbb{R}} \) and \( (s + r) \in \mathbb{R} \). In the case \( (s - r) \in \mathbb{R} \) and \( (s + r) \in \mathbb{R} \), by introducing
\[ \frac{s+r}{2} = \beta \cos \gamma \quad q = e^{\beta \cos \gamma} e^{i\beta \sin \gamma} \]
\[ \frac{s-r}{2} = \beta \sin \gamma \quad p = e^{\beta \cos \gamma} e^{-i\beta \sin \gamma} \] (40)
(where \( \beta \) and \( \gamma \) are two independent real parameters), the spectrum of \( H \) is given by
\[ E = \frac{1}{2\mathcal{I}} e^{(2J-1)\beta \cos \gamma} \frac{\sin(J\beta \sin \gamma) \sin[(J + 1)\beta \sin \gamma]}{\sin^2(\beta \sin \gamma)} + E_0 \] (41)
Similarly, in the case \( (s - r) \in \mathbb{R} \) and \( (s + r) \in \mathbb{R} \), by putting
\[ \frac{s+r}{2} = \beta \cos \gamma \quad q = e^{\beta \cos \gamma} e^{+\beta \sin \gamma} \]
\[ \frac{s-r}{2} = \beta \sin \gamma \quad p = e^{\beta \cos \gamma} e^{-\beta \sin \gamma} \] (42)
(where here again \( \beta \) and \( \gamma \) are real), the eigenvalues of \( H \) are
\[ E = \frac{1}{2\mathcal{I}} e^{(2J-1)\beta \cos \gamma} \frac{\sinh(J\beta \sin \gamma) \sinh[(J + 1)\beta \sin \gamma]}{\sinh^2(\beta \sin \gamma)} + E_0 \] (43)
Both equations (41) and (43) can be rewritten in the form
\[ E = \frac{1}{2\mathcal{I}_\beta \gamma} \left( \sum_{n=0}^{\infty} d_n(\beta, \gamma)[C_2(su_2)]^n + [2C_1(u_1) + 1] \sum_{n=0}^{\infty} c_n(\beta, \gamma)[C_2(su_2)]^n \right) + E_0 \] (44)
where
\[ I_{\beta,\gamma} = I e^{2\beta \cos \gamma} \]
\[ C_2(\text{su}_2) = J(J + 1) \]
\[ C_1(u_1) = J \quad (45) \]

The expansion coefficients \( c_n(\beta, \gamma) \) and \( d_n(\beta, \gamma) \) in (44) are given by series involving special functions.

The model inherent to formula (38) gives back the rigid rotor model in the limiting situation where \( p = q^{-1} = 1 \). The model corresponding to \( p^{-1} = q = e^{i\beta} \) (\( \beta \in \mathbb{R} \)) was introduced by Raychev et al. [23] for describing rotational bands of deformed and superdeformed nuclei. The more general two-parameter model corresponding to \( q = \bar{p} = e^{\beta \cos \gamma} e^{i\beta \sin \gamma} \) [see formula (41)] has been successfully applied to some superdeformed bands of even-even nuclei in the \( A \sim 190 \) region [24]; it has been shown in Ref. [24] that the introduction of a second parameter of a “quantum algebra” nature increases the agreement between theory and experiment in a significant way. Some tests for the application of the two-parameter model (39) [in the versions (41) and (43)] to molecules are presently under consideration.

6. Concluding remarks

From the applications described in sections 2 to 5, we can make the following comments.

They are several ways to obtain a \( q \)- (or \( qp \))-quantization of a given dynamical system.

(i) We may start from the connection (if it is known) between this system and oscillator systems, for which there is a (generally well accepted) consensus on the way to \( q \)-quantize them.

(ii) Another approach consists in replacing the dynamical invariance (Lie) algebra \( g \) of the considered system by a quantum algebra \( U_q(g) \).

(iii) We can also try to convert the Schrödinger (or Dirac) equation for the dynamical system into an equation involving \( q \)-derivative.

Of course, there is no reason to obtain the same \( q \)-quantized system from the approaches (i) to (iii). It is even possible to obtain two different \( q \)-quantized systems when working inside a given approach. (This is the case for the hydrogen atom for example.)

Similar remarks may be done about the derivation of a \( q \)-analogue of a given physical model.

The lack of unicity in deriving \( q \)-deformed objects is obviously a source of
pessimism in applications of quantum algebras to physics.

Another major drawback is the impossibility to obtain a universal significance of the deformation parameter $q$. For instance, $q$ may be connected to the fine structure constant for the hydrogen atom [14], to the softness parameter in rotational spectroscopy of nuclei [23], and to the chemical potential in Bose-Einstein statistics [25]. Furthermore, the parameter $q$, although useful from a phenomenological point of view, may have no physical significance. This is the case for the classification of chemical elements [22] or for the formation of coherent structures in strongly interacting $q$-boson systems [26].

Finally, in many cases, the results afforded by a $q$-quantization of a given model can be equally well obtained from an extension (out of the quantum algebra context) of the model.

The balance between optimism and pessimism seems to go towards pessimism. “What is the use of quantum groups? [27]” That is the question we have to face.

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