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LETTER TO THE EDITOR

Two models of a q-deformed hydrogen atom

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Abstract. Two possible methods of deformation of a hydrogen-like system in terms of the q-(deformed) boson operators are constructed. In the first case the system has $SU_q(2)\otimes SU_q(2)$ symmetry, while in the second $S(\otimes_{i=1}^{4} U_q(1))$ symmetry. The energy level degeneracy and splitting for both cases are explicitly calculated.

The theory of quantum algebras (deformations of quantum universal enveloping algebras) and quantum groups has several applications in a wide range of physical domains (statistical mechanics and solvable models [2], rational conformal field theory [1]). The nuclear rotational spectroscopy [4, 6] and atomic spectroscopy [14, 15] still attract much attention.

The q-analogue of the hydrogen atom has been investigated recently by Kibler and Negadi [14]. They considered a deformation of the Pauli equations as well as applying the Kustaanheimo–Stiefel (KS) transformation to achieve an alternative result. Those models possess the $SU_q(2)\otimes SU_q(2)$ and $SU_q(4)$ symmetry respectively. The 2s–2p Dirac shift was proposed by these authors in the context of the $SU_q(4)$ model; however, constraints connected to the 'usual' $(q=1)$ KS transformation were not taken into account. Thus, the energy levels of this model were not in agreement with the ones in a quantum mechanical limit.

On the other hand, Xing-Chang Song and Li Liao [15] used another way to approach the subject which employs non-commutative differential calculus on the quantum orthogonal planes. They solved the deformed version of the Schrödinger equation for the attractive Coulomb potential $V=-e^2/r$ and showed that the energy eigenvalues are proportional to $[n]^{-2}$ (where [ ] denotes a q-number $[n]=(q^n-q^{-n})/(q-q^{-1})$).

The aim of this letter is to strictly obtain the discrete spectrum $(E<0)$ of the q-(deformed) hydrogen atom using the connection between this and a q-quantum, d-dimensional harmonic oscillator given by the KS transformation. The approach in this letter is twofold: it allows us to introduce the $SU_q(2)\otimes SU_q(2)$ symmetry group of the q-hydrogen atom as well as to show an alternative $S(\otimes_{i=1}^{4} U_q(1))$ model. To this end we start with the q-quantum version of a 'usual' $SU(d)$ symmetry Hamiltonian:

$$h=\tfrac{1}{2}\sum_{i=1}^{d}(A_i\overset{+}{A}_i+\overset{+}{A}_iA_i) \tag{1}$$

where $[A_i, \overset{+}{A}_j]=1$. The prescription of a q-deformation of the quantum mechanical oscillator is well known at the moment in contrast to other physical objects where there does not exist a simple correspondence between q-deformed and 'usual' descriptions (e.g. [5]). Hence, we will construct two possible q-quantum versions of (1) in terms of the q-boson operators. Then, we will employ these results to the KS-transformed Schrödinger equation of the hydrogen atom.

The description of that transformation which boils down to the following $\{x_i: i=1,2,3\}\in R^3\to R^4\ni\{u_\alpha:\alpha=1,2,3,4\}$ surjection

$$\begin{aligned} x_1&=u_1^2-u_2^2-u_3^2+u_4^2\\ x_2&=2(u_1u_2-u_3u_4)\\ x_3&=2(u_1u_3+u_2u_4)\\ r&=\left(\sum_{i=1}^{3}x_i^2\right)^{1/2}=\sum_{\alpha=1}^{4}u_\alpha^2 \end{aligned}\tag{2}$$

as well as its application to the 'usual' hydrogen-like systems, has received a great deal of attention [3, 7, 8, 12, 13, 16]. The surjection (2) enables us to write the Schrödinger equation as the R^4 partial differential equation [14]:

$$(-(1/2\mu)\Delta_u+(1/2\mu r)R-4Ze^2)|\Psi\rangle=4rE|\Psi\rangle\tag{3}$$

with reduced mass μ and nucleus charge Ze, where

$$\Delta_u=\sum_{\alpha=1}^{4}\partial_\alpha^2=-\sum_{\alpha=1}^{4}P_\alpha^2\qquad R=u_4\partial_1-u_3\partial_2+u_2\partial_3-u_1\partial_4.\tag{4}$$

The operator R turns out to be an infinitesimal operator of a subgroup U(1) of a group O(4). Since we require the wavefunction $\langle u|\Psi\rangle$ to be univalued the condition $R|\Psi\rangle=0$ has to be fulfilled [3]. For our purpose the canonical transformation $\{u_\alpha, P_\alpha\}\to\{x_\alpha, p_\alpha\}$ [12] can be involved. Thus we arrive at the Schrödinger equation of a four-dimensional harmonic oscillator ($E<0$):

$$\left(-\frac{1}{2M}\sum_{\alpha=1}^{4}p_\alpha^2+\frac{M\omega^2}{2}\sum_{\alpha=1}^{4}x_\alpha^2\right)|\Psi\rangle=\left(\frac{4Ze^2}{\sqrt{-E}}\right)|\Psi\rangle\tag{5}$$

supplemented by the additional constraint relation

$$\left(\frac{1}{2M}(p_1^2+p_2^2-p_3^2-p_4^2)+\frac{M\omega^2}{2}(x_1^2+x_2^2-x_3^2-x_4^2)\right)|\Psi\rangle=0\tag{6}$$

where $M=\mu\sqrt{-E}$, $\mu\omega^2=1$.

Let us focus on the two q-analogues of the Hamiltonian (1). As it is well known, the q-deformed boson operators satisfy the following relations (e.g. [10, 11]):

$$\begin{aligned} &a_i\overset{+}{a}_j-q^{\delta_{ij}}\overset{+}{a}_ja_i=\delta_{ij}q^{-N_i}\\ &[N_i,N_j]=[\overset{(+)}{a}_i,\overset{(+)}{a}_j]=0\qquad [N_i]=\overset{+}{a}_ia_i\\ &[N_i,\overset{+}{a}_j]=\delta_{ij}\overset{+}{a}_i\\ &[N_i,a_j]=-\delta_{ij}a_i\qquad i,j=1,2,3,\ldots,d. \end{aligned}\tag{7}$$

The q-Fock space $\mathscr{H}_F$ is spanned by

$$\begin{aligned}\mathscr{H}_F=\mathrm{span}\{&|n_1,n_2,\ldots,n_d\rangle=([n_1]!\ldots[n_d]!)^{-1/2}\overset{+}{a}{}^{n_1}\ldots\overset{+}{a}{}^{n_d}|0\rangle:\\ &a_i|0\rangle=0,\ N_i|n_1,\ldots,n_d\rangle=n_i|n_1,\ldots,n_d\rangle\quad\forall i=1,\ldots,d\}\end{aligned}\tag{8}$$

where $[n]=(q^n-q^{-n})/(q-q^{-1})$.

Taking into consideration the idea given by Floratos [9] (i.e. 'q-summation rule') to the construction of the q-deformed $SU_q(d)$ variant of the oscillator we arrive at the q-Hamiltonian:

$$H_q = \frac{1}{2} \sum_{\varepsilon=\mp 1} \left[\sum_{i=1}^{d} N_i + \frac{(1+\varepsilon)d}{2} \right] \tag{9}$$

which is diagonal on $\mathscr{H}_F$.

As in the one-dimensional case the energy levels consist of two terms

$$E^q_{(n)} = E^q_{(n),+1} + E^q_{(n),-1} \qquad E^q_{(n),1} = E^q_{(n+d),-1} \qquad (n) = n_1 + \ldots + n_d \tag{10}$$

with either even and odd numbers of excitations ($d = 1(\text{mod}\,2)$) or the same parity ($d = 2(\text{mod}\,2)$). For the q-system described by (8), as long as (n) is fixed, the energy levels $E^q_{(n)}$ are degenerated. The degree of degeneracy equals the 'usual' one which is given by the number of partitions of $(n)+d$ into integers:

$$\deg E^q_{(n),\varepsilon} = \binom{(n)+d-1}{d-1}. \tag{11}$$

On the other hand the q-analogues of the d-dimensional oscillator can be achieved by considering d copies of a free q-oscillator:

$$\tilde{H}_q = \frac{1}{2} \sum_{i=1}^{d} \sum_{\varepsilon=\pm 1} \left[N_i + \frac{1+\varepsilon}{2} \right]. \tag{12}$$

In the Fock space (8) the eigenvalues of (12) are:

$$\begin{aligned} \tilde{E}^q_{(n)} &= \sum_{\varepsilon=\mp 1} \tilde{E}^q_{(n),\varepsilon} \qquad (n) = n_1 + \ldots + n_d \\ \tilde{E}^q_{(n),\varepsilon} &= \frac{1}{2} \sum_{i=1}^{d} \left[n_i + \frac{1+\varepsilon}{2} \right]. \end{aligned} \tag{13}$$

In contrast to the first case, since (n) is fixed, each energy level $\tilde{E}^q_{(n),\varepsilon}$ splits into $\mathfrak{P}((n)+d, d)$ levels

$$\tilde{E}^q_{(n),\varepsilon} = \sum_{i=1}^{d} \sum_{\max(n_i)<(n)} \tilde{E}^q_{(n,\max n_i),\varepsilon} \tag{14}$$

distinguished in addition by the number $\max(n_i) = \max\{n_1, \ldots, n_d\}$ for each $n_i < (n)$. The number $\mathfrak{P}((n)+d, d)$ is a number of partitions of $((n)+d)$ into d integers where partitions which differ only in an order of components are identified:

$$\mathfrak{P}(m, d) = \langle m^{d-1}/((d-1)!\,d!) + R_{(d-2)}(m) \rangle \tag{15}$$

where $\langle x \rangle$ denotes the integer nearest to x and $R_{(d-2)}(m)$ is the polynomial of the variable m and a degree no greater than $(d-2)$ with coefficients being functions of the rest $m(\text{mod}\, d!)$. So, to define (15) for a d-dimensional q-oscillator, $d!$ polynomials are indispensable, e.g.

$$\mathfrak{P}((n)+2, 2) = \begin{cases} \langle ((n)+2)/2 \rangle & (n) = 0(\text{mod}\,2), \\ \langle ((n)+1)/2 \rangle & (n) = 1(\text{mod}\,2). \end{cases} \tag{16}$$

Each one of the energy levels $\tilde{E}^q_{(n,\max n_i),\varepsilon}$ is degenerated. The degree of degeneracy of the level labelled with $((n), \max n_i)$ such that $n_1 = n_2 = \ldots = n_k$, $k \leqslant d$, is:

$$\deg \tilde{E}^q_{(n,\max n_i),\varepsilon} = \binom{d}{k} \tag{17}$$

and the distance

$$\Delta^{\varepsilon}_{(n,n-1)} := \tilde{E}^{q}_{(n,\max n_i),\varepsilon} - \tilde{E}^{q}_{(n-1,\max(n_i-1)),\varepsilon} \tag{18}$$

is given by:

$$\Delta^{\varepsilon}_{(n,n-1)} = \cosh s(\max(n_i-1)) \qquad q = e^{s}. \tag{19}$$

At this point, we are ready to show how our two models of the q-deformed oscillator could be connected with the q-deformed hydrogen-like system. To this end we construct q-versions of equations (5) and (6) according to both ways presented above. Therefore we get:

$$E^{q}_{(n_1,n_2,n_3,n_4)} = E^{q}_{0}\left(\left[\sum_{i=1}^{4} N_i\right] + \left[\sum_{i=1}^{4} N_i + 4\right]\right)^{-2} \tag{20}$$

$$\tilde{E}^{q}_{(n_1,n_2,n_3,n_4)} = \tilde{E}^{q}_{0}\left(\sum_{i=1}^{4} ([N_i] + [N_i+1])\right)^{-2} \tag{21}$$

as the solutions accompanied by the auxiliary conditions

$$[N_1 + N_2]|n\rangle = [N_3 + N_4]|n\rangle \tag{22}$$

$$\left\{\sum_{i=1}^{2} ([N_i] + [N_i+1])\right\}|n\rangle = \left\{\sum_{i=3}^{4} ([N_i] + [N_i+1])\right\}|n\rangle \tag{23}$$

respectively, where

$$p_\alpha = (2M\omega)^{1/2}(a - \overset{+}{a})/2\mathrm{i} \qquad x_\alpha = (2/M\omega)^{1/2}(a + \overset{+}{a})/2 \tag{24}$$

have been introduced. The solution (21) of the q-deformed, κs transformed Schrödinger equation has been given recently by Kibler and Negadi [14]. Using the same transformation and the q-deformed versions (22) and (23) of the 'usual' constraints [13] we get, in addition, an alternative result (20). These 'q-constraints' enable us to rewrite the spectra (20) and (21) as follows:

$$E^{q}_{(n_1,n_2)} = E^{q}_{0}([2(n_1+n_2)] + [2(n_1+n_2+2)])^{-2} \tag{25}$$

$$\tilde{E}^{q}_{(n_1,n_2)} = \tilde{E}^{q}_{0}\left(\sum_{i=1}^{2} ([n_i] + [n_i+1])\right)^{-2} \tag{26}$$

where $E^{q}_{0} = (16/[4]^2)\tilde{E}^{q}_{0} = -(Z^2 e^4 16)/[4]^2$.

The above equations describe inequivalent systems (as long as $q \neq 1$). The condition (22) implies the $\mathrm{SU}_q(2)\otimes\mathrm{SU}_q(2)$ symmetry of the hydrogen atom while the conditions (23) symmetry given by a product $\mathrm{S}(\otimes_{i=1}^{4} \mathrm{U}_q(1))$ which, in contrast to the 'usual' case, are not isomorphic to each other (e.g. [9]).

Using (11) and (17) one can obtain the degree of degeneracy of the energy levels

$$\deg E^{q}_{(n_1,n_2)} = (((n)+2)/2) \tag{27}$$

$$\deg \tilde{E}^{q}_{(n_1,n_2)} = \begin{cases} 4 & n_1 \neq n_2 \\ 1 & n_1 = n_2. \end{cases} \tag{28}$$

Introducing (16), the splitting of each $\tilde{E}^{q}_{(n_1+n_2)}$ level is given as $\{\mathfrak{P}((n_1+n_2+2),2)\}^2$.

To conclude we note that these descriptions of the q-quantum hydrogen-like system have interesting properties—the first one has the full 'classical' analogous, the second one is 2s–2p splittable without relativistic corrections (that has been underlined in

[14]). It seems to be worth pointing out the non-trivial role of the 'q-constraints' put into both cases on the system, especially because these admit the results which are in agreement not only with the 'classical' ($q=1$) limit but also with the q-spectra achieved by q-quantization of the Pauli equations [14] and by using the non-commutative differential calculus on the quantum orthogonal planes [6]. However, the unexpected splitting of the energy levels appears only in connection with the $S(\otimes_{i=1}^{4} U_q(1))$ symmetry of the q-hydrogen atom.

To sum up, we can say that only further phenomenological data investigations should lead to a clear conclusion about which q-quantum mechanics appears to be 'more reasonable'.

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