QUANTUM ALGEBRAIC SYMMETRIES IN NUCLEI AND MOLECULES

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ABSTRACT

Various applications of quantum algebraic techniques in nuclear and molecular physics are briefly reviewed. Emphasis is put in the study of the symmetries of the anisotropic quantum harmonic oscillator with rational ratios of frequencies, which underly the structure of superdeformed and hyperdeformed nuclei, the Bloch–Brink \(\alpha\)-cluster model and possibly the shell structure in deformed atomic clusters.

1. Introduction

Quantum algebras [1,2] (also called quantum groups) are deformed versions of the usual Lie algebras, to which they reduce when the deformation parameter \(q\) is set equal to unity. Their use in physics became popular with the introduction [3–5] of the \(q\)-deformed harmonic oscillator as a tool for providing a boson realization of the quantum algebra \(\text{su}_q(2)\), although similar mathematical structures had already been known [6,7]. Initially used for solving the quantum Yang–Baxter equation, quantum algebras have subsequently found applications in several branches of physics, as, for example, in the description of spin chains, squeezed states, rotational and vibrational nuclear and molecular spectra, and in conformal field theories. By now several kinds of generalized deformed oscillators [8,9] and generalized deformed \(\text{su}(2)\) algebras [10–12] have been introduced.

The main applications of quantum algebraic techniques in nuclear physics include:

i) The \(\text{su}_q(2)\) rotator model, used for the description of rotational spectra of deformed [13,14] and superdeformed [15] nuclei, as well as for the description of the electromagnetic transition probabilities [16] connecting the energy levels within each band.

ii) Extensions of the \(\text{su}_q(2)\) model suitable for the description of vibrational and transitional nuclear spectra [17].

iii) Generalized deformed \(\text{su}_\Phi(2)\) algebras [10], characterized by a structure function \(\Phi\) and possessing a representation theory similar to that of the usual \(\text{su}(2)\) algebra. The \(\text{su}_q(2)\) algebra occurs for a special choice of \(\Phi\), while different choices lead to different energy formulae for the rotational spectrum, as, for example, the Holmberg–Lipas formula [18].

iv) The use of deformed bosons for the description of pairing correlations in nuclei [19–21].

v) The construction of deformed versions of various exactly soluble models, as the Interacting Boson Model [22] and the Moszkowski model [23]. In the framework of the latter, RPA modes [24] and high spin states [25] have also been studied.
vi) The study of the symmetries of the anisotropic quantum harmonic oscillator with rational ratios of frequencies (RHO), which are of interest in connection with superdeformed and hyperdeformed nuclei [26,27], “pancake” nuclei (i.e. very oblate nuclei) [27], cluster configurations in light nuclei [28] connected to the Bloch–Brink α cluster model [29], and possibly in connection with deformed atomic clusters [30,31].

The main applications of quantum algebraic techniques in molecular physics include:

i) The su_q(2) rotator model, used for the description of rotational spectra of diatomic molecules [32].

ii) The description of vibrational spectra of diatomic molecules in terms of the su_q(1,1) algebra [33,34], as well as in terms of generalized deformed oscillators [35]. WKB equivalent potentials possessing the same spectrum as these oscillators have also been constructed [36]. These oscillators have been found appropriate for approximating certain Quasi Exactly Soluble Potentials [37].

iii) The development of a deformed version of the vibron model [38] of molecular structure.

iv) The construction of deformed oscillators equivalent to the Morse potential [39] and the use of a set of such oscillators for the description of the vibrational spectra of highly symmetric polyatomic molecules [40].

In the remainder of this paper the symmetries of the anisotropic quantum harmonic oscillator with rational ratios of frequencies will be considered in more detail.

2. Anisotropic quantum harmonic oscillator with rational ratios of frequencies

The symmetries of the 3-dimensional anisotropic quantum harmonic oscillator with rational ratios of frequencies (RHO) are of high current interest in nuclear physics, since they are the basic symmetries underlying the structure of superdeformed and hyperdeformed nuclei [26,27]. The 2-dimensional RHO is also of interest, in connection with “pancake” nuclei, i.e. very oblate nuclei [27]. Cluster configurations in light nuclei can also be described in terms of RHO symmetries [28], which underlie the geometrical structure of the Bloch–Brink α-cluster model [29]. The 3-dim RHO is also of interest for the interpretation of the observed shell structure in atomic clusters [30], especially after the realization [31] that large deformations can occur in such systems.

The two-dimensional [41,42] and three-dimensional [43,44] anisotropic harmonic oscillators have been the subject of several investigations, both at the classical and the quantum mechanical level. These oscillators are examples of superintegrable systems [45]. The special cases with frequency ratios 1:2 [46] and 1:3 [47] have also been considered. While at the classical level it is clear that the su(N) or sp(2N,R) algebras can be used for the description of the N-dimensional anisotropic oscillator, the situation at the quantum level, even in the two-dimensional case, is not as simple.

In the remainder of this section the 2-dim RHO will be considered in more detail.

2.1. The deformed u(2) algebra

Let us consider the system described by the Hamiltonian:

$$H = \frac{1}{2} \left( p_x^2 + p_y^2 + \frac{x^2}{m^2} + \frac{y^2}{n^2} \right),$$

(1)
where $m$ and $n$ are two natural numbers mutually prime ones, i.e. their great common divisor is $\gcd(m, n) = 1$.

We define the creation and annihilation operators \[41\]

\[
a^\dagger = \frac{x/m - ipx}{\sqrt{2}}, \quad a = \frac{x/m + ipx}{\sqrt{2}}, \quad b^\dagger = \frac{y/n -ipy}{\sqrt{2}}, \quad b = \frac{y/n + ipy}{\sqrt{2}}. \tag{2}
\]

These operators satisfy the commutation relations:

\[
[a, a^\dagger] = \frac{1}{m}, \quad [b, b^\dagger] = \frac{1}{n}, \quad \text{other commutators} = 0. \tag{3}
\]

One can further define

\[
U = \frac{1}{2} \{a, a^\dagger\}, \quad W = \frac{1}{2} \{b, b^\dagger\}.
\]

One can then define the enveloping algebra generated by the operators:

\[
S_+ = (a^\dagger)^m (b)^n, \quad S_- = (a)^m (b^\dagger)^n,
\]

\[
S_0 = \frac{1}{2} (U - W), \quad H = U + W.
\]

These generators satisfy the following relations:

\[
[S_0, S_i] = \pm S_i, \quad [H, S_i] = 0, \quad \text{for} \quad i = 0, \pm, \tag{5}
\]

and

\[
S_+ S_- = \prod_{k=1}^{m} \left( U - \frac{2k-1}{2m} \right) \prod_{\ell=1}^{n} \left( W + \frac{2\ell - 1}{2n} \right),
\]

\[
S_- S_+ = \prod_{k=1}^{m} \left( U + \frac{2k-1}{2m} \right) \prod_{\ell=1}^{n} \left( W - \frac{2\ell - 1}{2n} \right).
\]

The fact that the operators $S_i$, $i = 0, \pm$ are integrals of motion has been already realized in \[41\].

The above relations mean that the harmonic oscillator of Eq. (1) is described by the enveloping algebra of the generalization of the $u(2)$ algebra formed by the generators $S_0$, $S_+$, $S_-$ and $H$, satisfying the commutation relations of Eq. (5) and

\[
[S_- S_+] = F_{m,n}(H, S_0 + 1) - F_{m,n}(H, S_0), \tag{6}
\]

where

\[
F_{m,n}(H, S_0) = \prod_{k=1}^{m} \left( H/2 + S_0 - \frac{2k-1}{2m} \right) \prod_{\ell=1}^{n} \left( H/2 - S_0 + \frac{2\ell - 1}{2n} \right).
\]

In the case of $m = 1, n = 1$ this algebra is the usual $u(2)$ algebra, and the operators $S_0, S_\pm$ satisfy the commutation relations of the ordinary $u(2)$ algebra, since in this case one easily finds that

\[
[S_- S_+] = -2S_0.
\]
In the rest of the cases, the algebra is a deformed version of $u(2)$, in which the commutator $[S_-, S_+]$ is a polynomial of $S_0$ of order $m + n - 1$.

2.2. The representations

The finite dimensional representation modules of this algebra can be found using the concept of the generalized deformed oscillator [8], in a method similar to the one used in [48] for the study of quantum superintegrable systems. The operators:

$$A^\dagger = S_+, \quad A = S_-, \quad \mathcal{N} = S_0 - u, \quad u = \text{constant},$$

where $u$ is a constant to be determined, are the generators of a deformed oscillator algebra:

$$[\mathcal{N}, A^\dagger] = A^\dagger, \quad [\mathcal{N}, A] = -A, \quad A^\dagger A = \Phi(H, \mathcal{N}), \quad AA^\dagger = \Phi(H, \mathcal{N} + 1).$$

The structure function $\Phi$ of this algebra is determined by the function $F_{m,n}$ in Eq. (6):

$$\Phi(H, \mathcal{N}) = F_{m,n}(H, \mathcal{N} + u) = \prod_{k=1}^{m} \left(\frac{H}{2} + \mathcal{N} + u - \frac{2k-1}{2m}\right) \prod_{\ell=1}^{n} \left(\frac{H}{2} - \mathcal{N} - u + \frac{2\ell-1}{2n}\right).$$

The deformed oscillator corresponding to the structure function of Eq. (8) has an energy dependent Fock space of dimension $\mathcal{N} + 1$ if

$$\Phi(E, 0) = 0, \quad \Phi(E, \mathcal{N} + 1) = 0, \quad \Phi(E, k) > 0, \quad \text{for} \quad k = 1, 2, \ldots, \mathcal{N}. \quad (9)$$

The Fock space is defined by:

$$H|E, k >= E|E, k >, \quad \mathcal{N}|E, k >= k|E, k >, \quad a|E, 0 >= 0,$$

$$A^\dagger|E, k >= \sqrt{\Phi(E, k + 1)}|E, k + 1 >, \quad A|E, k >= \sqrt{\Phi(E, k)}|E, k - 1 >. \quad (11)$$

The basis of the Fock space is given by:

$$|E, k >= \frac{1}{\sqrt{[k]!}} \left(\mathcal{A}^\dagger\right)^k |E, 0 >, \quad k = 0, 1, \ldots N,$$

where the “factorial” $[k]!$ is defined by the recurrence relation:

$$[0]! = 1, \quad [k]! = \Phi(E, k)[k - 1]!.$$

Using the Fock basis we can find the matrix representation of the deformed oscillator and then the matrix representation of the algebra of Eqs (5), (6). The solution of Eqs (9) implies the following pairs of permitted values for the energy eigenvalue $E$ and the constant $u$:

$$E = N + \frac{2p - 1}{2m} + \frac{2q - 1}{2n}, \quad (12)$$
where \( p = 1, 2, \ldots, m \), \( q = 1, 2, \ldots, n \), and

\[
u = \frac{1}{2} \left( \frac{2p - 1}{2m} - \frac{2q - 1}{2n} - N \right),
\]

the corresponding structure function being given by:

\[
\Phi(E, x) = \Phi^N_{(p, q)}(x) = \prod_{k=1}^{m} \left( x + \frac{2p - 1}{2m} - \frac{2k - 1}{2m} \right) \prod_{\ell=1}^{n} \left( N - x + \frac{2q - 1}{2n} + \frac{2\ell - 1}{2n} \right)
\]

(13)

\[
eq \frac{1}{m^m n^n} \frac{\Gamma((N-x)n+q+n)}{\Gamma((N-x)n+q)}.\]

In all these equations one has \( N = 0, 1, 2, \ldots \), while the dimensionality of the representation is given by \( N+1 \). Eq. (12) means that there are \( m \cdot n \) energy eigenvalues corresponding to each \( N \) value, each eigenvalue having degeneracy \( N+1 \). (Later we shall see that the degenerate states corresponding to the same eigenvalue can be labelled by an “angular momentum”.)

The energy formula can be corroborated by using the corresponding Schrödinger equation. For the Hamiltonian of Eq. (1) the eigenvalues of the Schrödinger equation are given by:

\[
E = \frac{1}{m} \left( n_x + \frac{1}{2} \right) + \frac{1}{n} \left( n_y + \frac{1}{2} \right),
\]

(14)

where \( n_x = 0, 1, \ldots \) and \( n_y = 0, 1, \ldots \). Comparing Eqs (12) and (14) one concludes that:

\[
N = [n_x/m] + [n_y/n],
\]

where \([x]\) is the integer part of the number \( x \), and

\[
p = \text{mod}(n_x, m) + 1, \quad q = \text{mod}(n_y, n) + 1.
\]

The eigenvectors of the Hamiltonian can be parametrized by the dimensionality of the representation \( N \), the numbers \( p, q \), and the number \( k = 0, 1, \ldots, N \). \( k \) can be identified as \([n_x/m]\). One then has:

\[
H \left| \begin{array}{c} N \\ (p, q), k \end{array} \right> = \left( N + \frac{2p - 1}{2m} + \frac{2q - 1}{2n} \right) \left| \begin{array}{c} N \\ (p, q), k \end{array} \right>,
\]

(15)

\[
S_0 \left| \begin{array}{c} N \\ (p, q), k \end{array} \right> = \left( k + \frac{1}{2} \left( \frac{2p - 1}{2m} - \frac{2q - 1}{2n} - N \right) \right) \left| \begin{array}{c} N \\ (p, q), k \end{array} \right>,
\]

(16)

\[
S_+ \left| \begin{array}{c} N \\ (p, q), k \end{array} \right> = \sqrt{\Phi^N_{(p, q)}(k+1)} \left| \begin{array}{c} N \\ (p, q), k+1 \end{array} \right>,
\]

(17)

\[
S_- \left| \begin{array}{c} N \\ (p, q), k \end{array} \right> = \sqrt{\Phi^N_{(p, q)}(k)} \left| \begin{array}{c} N \\ (p, q), k-1 \end{array} \right>.
\]

(18)

2.3. The “angular momentum” quantum number
It is worth noticing that the operators $S_0, S_\pm$ do not correspond to a generalization of the angular momentum, $S_0$ being the operator corresponding to the Fradkin operator $S_{xx} - S_{yy}$ [49]. The corresponding “angular momentum” is defined by:

$$L_0 = -i \left( S_+ - S_- \right).$$

(19)

The “angular momentum” operator commutes with the Hamiltonian:

$$[H, L_0] = 0.$$

Let $|\ell\rangle$ be the eigenvector of the operator $L_0$ corresponding to the eigenvalue $\ell$. The general form of this eigenvector can be given by:

$$|\ell\rangle = \sum_{k=0}^{N} \frac{i^k c_k}{\sqrt{|k|!}} N_{(p,q),k}. \tag{20}$$

In order to find the eigenvalues of $L$ and the coefficients $c_k$ we use the Lanczos algorithm, as formulated in [50]. From Eqs (17) and (18) we find

$$L_0 |\ell\rangle = \ell |\ell\rangle = \sum_{k=0}^{N} \frac{i^k c_k}{\sqrt{|k|!}} N_{(p,q),k} = \frac{1}{\sqrt{2}} \sum_{k=0}^{N-1} \frac{i^k c_k}{\sqrt{|k|!}} \Phi^N_{(p,q),k+1} - \frac{1}{\sqrt{2}} \sum_{k=1}^{N} \frac{i^k c_k}{\sqrt{|k|!}} \Phi^N_{(p,q),k}.$$ 

From this equation we find that:

$$c_k = (-1)^k 2^{-k/2} H_k(\ell/\sqrt{2})/N, \quad N^2 = \sum_{n=0}^{N} 2^{-n} H_n^2(\ell/\sqrt{2})$$

where the function $H_k(x)$ is a generalization of the “Hermite” polynomials (see also [51,52]), satisfying the recurrence relations:

$$H_{-1}(x) = 0, \quad H_0(x) = 1,$$

$$H_{k+1}(x) = 2x H_k(x) - 2\Phi^N_{(p,q),k} H_{k-1}(x),$$

and the “angular momentum” eigenvalues $\ell$ are the roots of the polynomial equation:

$$H_{N+1}(\ell/\sqrt{2}) = 0. \tag{21}$$

Therefore for a given value of $N$ there are $N + 1$ “angular momentum” eigenvalues $\ell$, symmetric around zero (i.e. if $\ell$ is an “angular momentum” eigenvalue, then $-\ell$ is also an “angular momentum” eigenvalue). In the case of the symmetric harmonic oscillator ($m/n = 1/1$) these eigenvalues are uniformly distributed and differ by 2. In the general case the “angular momentum” eigenvalues are non-uniformly distributed. For small values of $N$ analytical formulae for the “angular momentum” eigenvalues can be found [51]. Remember that to each value of $N$ correspond $m \cdot n$ energy levels, each with degeneracy $N + 1$. 
In order to have a formalism corresponding to the one of the isotropic oscillator, let us introduce for every $N$ and $(p,q)$ an ordering of the “angular momentum” eigenvalues

$$\ell_m^{L,(p,q)}, \quad \text{where} \quad L = N \quad \text{and} \quad m = -L, -L+2, \ldots, L-2, L,$$

by assuming that:

$$\ell_m^{L,(p,q)} \leq \ell_n^{L,(p,q)} \quad \text{if} \quad m < n,$$

the corresponding eigenstate being given by:

$$|L, m; (p, q)\rangle = \sum_{k=0}^{N} \frac{(-i)^k H_k(\ell_m^{L,(p,q)}/\sqrt{2})}{N \sqrt{2^k/k!}} \left| N - k \right\rangle .$$  \(22\)

The above vector elements constitute the analogue corresponding to the basis of “spherical harmonic” functions of the usual oscillator.

2.4. Summary

In conclusion, the two-dimensional anisotropic quantum harmonic oscillator with rational ratio of frequencies equal to $m/n$, is described dynamically by a deformed version of the $u(2)$ Lie algebra, the order of this algebra being $m + n - 1$. The representation modules of this algebra can be generated by using the deformed oscillator algebra. The energy eigenvalues are calculated by the requirement of the existence of finite dimensional representation modules. An “angular momentum” operator useful for labelling degenerate states has also been constructed.

The extension of the present method to the three-dimensional anisotropic quantum harmonic oscillator is already receiving attention, since it is of clear interest in the study of the symmetries underlying the structure of superdeformed and hyperdeformed nuclei.

3. References

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