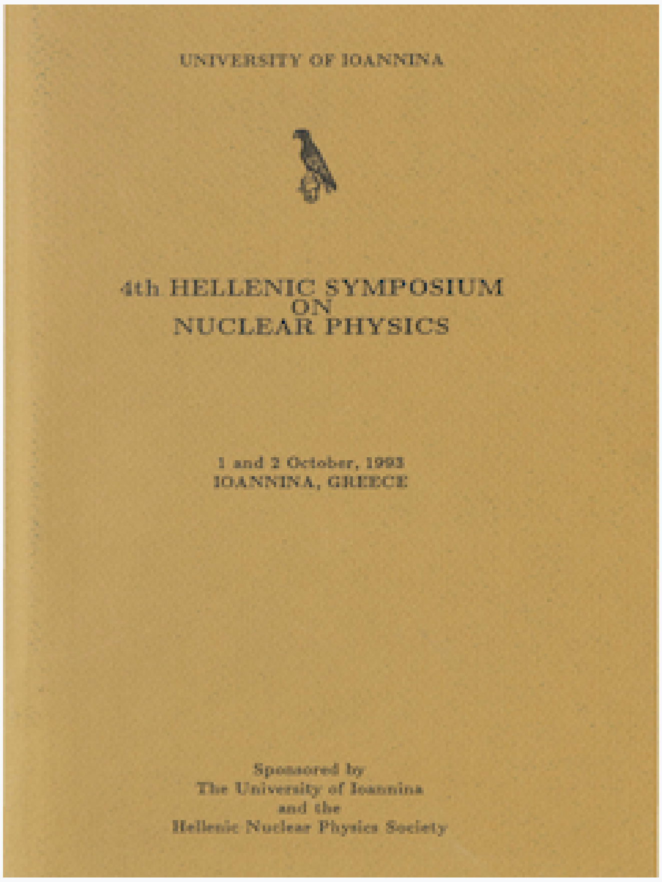
HNPS Advances in Nuclear Physics

Vol 4 (1993)

HNPS1993



UNIVERSITY OF IOANNINA

4th HELLENIC SYMPOSIUM
ON
NUCLEAR PHYSICS

1 and 2 October, 1993
IOANNINA, GREECE

Sponsored by
The University of Ioannina
and the
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doi: 10.12681/hnps.2879

To cite this article:

Bonatsos, D., & Daskaloyannis, C. (2020). Vibrational molecular and nuclear spectra in terms of quantum algebras. *HNPS Advances in Nuclear Physics*, *4*, 121–140. https://doi.org/10.12681/hnps.2879

VIBRATIONAL MOLECULAR AND NUCLEAR SPECTRA IN TERMS OF QUANTUM ALGEBRAS [1]

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Abstract

A generalized deformed oscillator giving the same spectrum as the Morse potential is constructed through the use of quantum algebraic techniques. The model of n coupled anharmonic oscillators of Iachello and Oss, suitable for the description of vibrational spectra of polyatomic molecules, is subsequently written in terms of such generalized deformed oscillators. In addition to clarifying the relation of the model of Iachello and Oss to other models using coupled oscillators for the description of vibrational molecular spectra, the present formalism allows for the construction of a large class of exactly soluble models with no extra computational effort. As an example, the way of including a coupling of the Darling-Dennison type is shown. Nuclear models giving good descriptions of vibrational spectra are reviewed and the need of modifying the $SU_q(2)$ model in order to extend its region of applicability towards the vibrational limit is discussed.

1. Introduction

Quantum algebras (also called quantum groups) [1], are receiving recently much attention in physics. From the mathematical point of view they are q-deformations of the universal

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[1] Presented by Dennis Bonatsos

enveloping algebras of the corresponding Lie algebras. When the deformation parameter q is set equal to 1, the usual Lie algebras are obtained. Quantum algebras are concrete examples of Hopf algebras. Initially used for solving the quantum Yang Baxter equation, they are now finding applications in several branches of physics, especially after the introduction of the q-deformed harmonic oscillator [2, 3]. Applications in conformal field theory, quantum gravity, quantum optics, supersymmetric quantum mechanics, superintegrable systems, atomic physics, as well as in the description of spin chains have already appeared (see [4] for relevant references).

Rotational spectra of diatomic molecules, deformed nuclei, and superdeformed nuclei have been described in terms of the q-deformed rotator having the symmetry $SU_q(2)$. The implications of this symmetry on the electric transition probabilities connecting the rotational levels have also been studied. A list of references is given in [4], where a generalization of the deformed SU(2) symmetry is discussed. Vibrational spectra of diatomic molecules have been described in terms of q-deformed harmonic [5, 6, 7, 8] and anharmonic [9, 10, 11] oscillators. WKB equivalent potentials for these oscillators have been determined [12, 13, 14], the WKB equivalent potential corresponding to the anharmonic oscillator with $SU_q(1,1)$ symmetry found [13] to be a deformation of the modified Pöschl-Teller potential, which is connected to the Morse potential by a known transformation [15].

On the other hand, a powerful method for the algebraic description of vibrational spectra of polyatomic molecules has been recently introduced by Iachello and Oss [16, 17, 18]. In this method, each bond in a polyatomic molecule is replaced by a Morse oscillator. The model is obviously superior in comparison to models attempting the description of vibrational spectra of polyatomic molecules in terms of coupled harmonic oscillators [19, 20, 21, 22], since it incorporates anharmonicities in a natural way. It is also much easier to use than the vibron model [23, 24], in which rotations and vibrations are treated simultaneously.

Since it is by now understood that the q-deformed oscillator is also a case of an anharmonic oscillator [25], it is reasonable to try to construct creation and annihilation operators describing a Morse oscillator, in a way similar to the description of the usual harmonic oscillator in the occupation number representation ("second quantization"). These operators can then be used in formulating the model of n coupled anharmonic oscillators of Iachello and Oss [16, 17, 18] in terms of deformed oscillators.

In section 2 of this paper we are going to construct creation and annihilation operators giving the same spectrum as the Morse potential. Subsequently, in section 3, the model of n coupled anharmonic oscillators of Iachello and Oss will be written in terms of these oscillators. In this way the relation of this model to existing models using coupled oscillators for the description of vibrational spectra of polyatomic molecules [19, 20, 21, 22] will be clarified. Furthermore, it will be demonstrated how a large class of exactly soluble models for the description of vibrations of polyatomic molecules can be constructed with no extra computational effort, by taking advantage of the freedom in the choice of the deformed oscillators involved and the simplicity of the occupation number representation formalism.

Finally, in section 4, the algebraic description of vibrational and transitional nuclear spectra will be discussed. The $\mathrm{SU}_q(2)$ model mentioned above ([4] and references therein) gives good results only in the rotational region, as expected. Physically motivated extensions of this model, aiming to extending its region of applicability towards the vibrational limit, will be discussed, based on the existing experience from other models.

2. A generalized deformed oscillator for the Morse potential

Solving the Schrödinger equation for the Morse potential [16, 26, 27]

$$V(x) = D\left(1 - e^{-\alpha x}\right)^2, \tag{1}$$

one obtains the energy spectrum

$$E(v) = -D - 4A(\mathcal{N}v - v^2), \tag{2}$$

where

$$v = 0, \quad 1, \quad \ldots, \quad \frac{\mathcal{N}}{2} \quad \text{or} \quad \frac{\mathcal{N}-1}{2} \quad (\mathcal{N} = \text{even} \quad \text{or} \quad \text{odd}), \tag{3}$$

and

$$-4A\mathcal{N} = \hbar\alpha\sqrt{\frac{2D}{m}}, \qquad 4A = -\frac{\hbar^2\alpha^2}{2m}. \tag{4}$$

The anharmonicity constant $x_e = 1/\mathcal{N}$, defined by Cooper [28], is a perturbational parameter for the Morse potential, measuring the deviation from the harmonic oscillator limit, which is obtained at $x_e \to 0$.

Our first aim is to construct a deformed oscillator giving the same spectrum as in eq. (2). Deformed oscillators giving the spectrum of a Pöschl-Teller potential have already been studied in [29], where the method of [30] was applied. This method gives the deformed oscillator directly from the energy spectrum. The Pöschl-Teller spectrum coincides with the spectrum of the Morse potential up to an energy shift, therefore the oscillator algebra of [29] can be transferred to the case of the Morse potential.

A general deformation of the harmonic oscillator can be given by the basic relation [30]

$$f(aa^+) - f(a^+a) = 1, \tag{5}$$

where a^+ (a) are creation (annihilation) operators and $f(x)$ is a real analytic function defined on the real positive axis. In the case of the usual harmonic oscillator one has $f(x) = x$, which leads to the usual boson commutation relation $[a, a^+] = 1$.

The number operator N satisfies, by definition, the commutation relations

$$[a, N] = a, \quad [a^+, N] = -a^+. \tag{6}$$

It can be shown [30] that

$$N = f(a^+a). \tag{7}$$

If (5) holds, then it is also true that

$$aa^+ = g(a^+a), \tag{8}$$

where the function $g(x)$ is defined by

$$g(x) = F(1 + f(x)), \quad F = f^{-1}. \tag{9}$$

If $|\alpha>$ is a base of eigenvectors of the number operator N

$$N|\alpha>= \alpha|\alpha>, \tag{10}$$

then from eq. (6) one has

$$a|\alpha>= \sqrt{[\alpha]}|\alpha - 1>, \quad a^+|\alpha>= \sqrt{[\alpha + 1]}|\alpha + 1>, \tag{11}$$

where $[\alpha]$ is a function of α. Furthermore from eq. (9) one has

$$[\alpha+1] = g([\alpha]), \quad or \quad f([\alpha+1]) = 1 + f([\alpha]), \tag{12}$$

from which we conclude that [45]

$$[\alpha] = F(\alpha). \tag{13}$$

The eigenvector $|0>$, corresponding to the zero eigenvalue of the number operator N, satisfies the following relation

$$\text{if} \quad F(0) = 0 \quad (\text{or} \quad f(0) = 0) \quad \text{then} \quad a|0>= 0. \tag{14}$$

In this paper we assume that the function $F(x)$ is zero when $x = 0$.

The number operator N defined by eq. (7) satisfies eqs. (6). The following identities are also useful:

$$a^+a = F(N) = [N], \qquad aa^+ = F(N+1) = [N+1], \tag{15}$$

and

$$\left[a, a^+\right] = [N+1] - [N], \qquad \left\{a, a^+\right\} = [N+1] + [N]. \tag{16}$$

If $h(z)$ is an entire function, then the following properties are true:

$$h(N)(a^+)^m = (a^+)^m h(N+m), \tag{17}$$

$$h(N+m)(a)^m = (a)^m h(N). \tag{18}$$

The eigenvectors of the number operator N are generated by the formula

$$|n>= \frac{1}{\sqrt{[n]!}}(a^+)^n|0>, \tag{19}$$

where

$$[n]! = \prod_{k=1}^{n}[k] = \prod_{k=1}^{n} F(k). \tag{20}$$

These eigenvectors are also eigenvectors of the energy operator

$$H = \frac{A}{2}(aa^+ + a^+a), \tag{21}$$

corresponding to the eigenvalues

$$E_n = \frac{A}{2}([n+1] + [n]) = \frac{A}{2}(F(n+1) + F(n)). \tag{22}$$

If the energy spectrum is given by a definite real function of the number $n + 1/2$

$$E_n = \frac{A}{2} H(n + \frac{1}{2}), \tag{23}$$

then

$$H(x + \frac{1}{2}) = \frac{1}{2}(F(x + 1) + F(x)). \tag{24}$$

The specific properties of the generalized deformed oscillator formulated above are fixed by the structure function $F(n)$. By choosing

$$F(n) = n, \tag{25}$$

one obtains the usual harmonic oscillator. For

$$F(n) = \frac{q^n - q^{-n}}{q - q^{-1}} = [n], \tag{26}$$

one obtains the q-deformed harmonic oscillator of Biedenharn [2] and Macfarlane [3], while by selecting

$$F(n) = \frac{Q^n - 1}{Q - 1} \tag{27}$$

the Q-deformed oscillator of Arik and Coon [31] can be generated. For $Q > 1$ the spectrum of this oscillator increases more rapidly than the equidistant spectrum of the usual harmonic oscillator, while for $Q < 1$ its spectrum increases less rapidly than equidistant, i.e. it is compressed, bearing similarity to the spectrum of the Morse oscillator.

We now look for a structure function which will give a spectrum similar to that of eq. (2). Since eq. (2) contains a polynomial quadratic in v and in addition we wish to keep $F(0) = 0$, the structure function should be of the form

$$F(V) = a_1 V + b_1 V^2. \tag{28}$$

Using eqs. (2) and (24) we easily conclude that a solution to the problem is provided by the structure function

$$F(V) = V(\mathcal{N} + 1 - V). \tag{29}$$

Using the basis $|\mathcal{N}, v>$ of eigenfunctions of the "number operator" V, one has in the place of eqs. (10), (11) the relations

$$V|\mathcal{N}, v> = v|\mathcal{N}, v>, \tag{30}$$

$$a|\mathcal{N},v> = \sqrt{F(v)}|\mathcal{N},v-1>, \qquad a^{+}|\mathcal{N},v> = \sqrt{F(v+1)}|\mathcal{N},v+1> . \tag{31}$$

The structure function of eq. (28) leads then to a spectrum

$$E'(v) = -4A\left(\frac{F(v)+F(v+1)}{2}\right) = -4A(\mathcal{N}v - v^2) - 2A\mathcal{N}. \tag{32}$$

Then eq. (2) can be written in the form

$$E(v) = E'(v) + 2A\mathcal{N} - D, \tag{33}$$

i.e. the spectrum of the generalized deformed oscillator constructed here is the same as the spectrum of the Morse potential up to an additive constant.

3. Model of n coupled generalized deformed oscillators

Iachello and Oss [16, 17, 18] introduced recently a model of n coupled anharmonic oscillators for the description of vibrational spectra of polyatomic molecules. In this model each bond i in a polyatomic molecule is replaced by a Morse oscillator. The model Hamiltonian has the form

$$H = E_0 + \sum_{i=1}^{n} A_i C_i + \sum_{i<j}^{n} A_{ij} C_{ij} + \sum_{i<j}^{n} \lambda_{ij} M_{ij}, \tag{34}$$

where C_i gives the spectrum of the ith Morse oscillator, while the interactions among the various Morse oscillators are described by C_{ij} and M_{ij}, the Casimir and Majorana interactions, respectively. The eigenvalues of C_i in the basis $|\mathcal{N}_i, v_i>$ are given by

$$<\mathcal{N}_i, v_i|C_i|\mathcal{N}_i, v_i> = -4(\mathcal{N}_i v_i - v_i^2). \tag{35}$$

The Casimir interaction C_{ij} is diagonal in the basis $|\mathcal{N}_i, v_i, \mathcal{N}_j, v_j>$, its matrix elements being

$$<\mathcal{N}_i, v_i, \mathcal{N}_j, v_j|C_{ij}|\mathcal{N}_i, v_i, \mathcal{N}_j, v_j> = 4((v_i+v_j)^2 - (v_i+v_j)(\mathcal{N}_i+\mathcal{N}_j)), \tag{36}$$

while the Majorana interaction M_{ij} has diagonal matrix elements

$$<\mathcal{N}_i, v_i, \mathcal{N}_j, v_j|M_{ij}|\mathcal{N}_i, v_i, \mathcal{N}_j, v_j> = v_i\mathcal{N}_j + v_j\mathcal{N}_i - 2v_iv_j, \tag{37}$$

and nondiagonal matrix elements

$$<\mathcal{N}_i, v_i+1, \mathcal{N}_j, v_j-1|M_{ij}|\mathcal{N}_i, v_i, \mathcal{N}_j, v_j>$$

$$= -\sqrt{u_j(v_i + 1)(\mathcal{N}_i - v_i)(\mathcal{N}_j - v_j + 1)}, \tag{38}$$

$$< \mathcal{N}_i, v_i - 1, \mathcal{N}_j, v_j + 1 | M_{ij} | \mathcal{N}_i, v_i, \mathcal{N}_j, v_j >$$

$$= -\sqrt{v_i(v_j + 1)(\mathcal{N}_j - v_j)(\mathcal{N}_i - v_i + 1)}. \tag{39}$$

We are now going to express these results in terms of the generalized deformed oscillator equivalent to the Morse potential, introduced in the previous section. Having in mind that

$$a_i^+ a_i = F(V_i), \qquad a_i a_i^+ = F(V_i + 1), \tag{40}$$

and noticing that

$$\{a_i, a_i^+\} | \mathcal{N}_i, v_i >= (F(V_i + 1) + F(V_i)) | \mathcal{N}_i, v_i >$$

$$= (2\mathcal{N}_i v_i - v_i^2 + \mathcal{N}_i) | \mathcal{N}_i, v_i >, \tag{41}$$

it is clear that the operator

$$C_i = 2(\mathcal{N}_i - \{a_i, a_i^+\}) = 2(\mathcal{N}_i - F(V_i) - F(V_i + 1)), \tag{42}$$

has the eigenvalues given in eq. (35).

Our next aim is to express the Casimir operator C_{ij} in terms of generalized oscillators. Noticing that

$$[a_i, a_i^+] | \mathcal{N}_i, v_i >= (F(V_i + 1) - F(V_i)) | \mathcal{N}_i, v_i >$$

$$= (\mathcal{N}_i - 2v_i) | \mathcal{N}_i, v_i >, \tag{43}$$

$$[a_i, a_i^+][a_j, a_j^+] | \mathcal{N}_i, v_i, \mathcal{N}_j, v_j >$$

$$= (F(V_i + 1) - F(V_i))(F(V_j + 1) - F(V_j)) | \mathcal{N}_i, v_i, \mathcal{N}_j v_j >$$

$$= (\mathcal{N}_i - 2v_i)(\mathcal{N}_j - 2v_j) | \mathcal{N}_i, v_i, \mathcal{N}_j, v_j >, \tag{44}$$

it is easy to verify that the operator

$$C_{ij} = 2(\mathcal{N}_i - \{a_i, a_i^+\} + \mathcal{N}_j - \{a_j, a_j^+\} - \mathcal{N}_i \mathcal{N}_j + [a_i, a_i^+][a_j, a_j^+]), \tag{45}$$

has the matrix elements given in eq. (36).

Finally, we wish to express the Majorana operator M_{ij} in terms of generalized oscillators. Noticing that

$$a_i^+ a_j|\mathcal{N}_i, v_i, \mathcal{N}_j, v_j >= \sqrt{F(V_i+1)F(V_j)}|\mathcal{N}_i, v_i+1, \mathcal{N}_j, v_j-1 >$$

$$= \sqrt{(v_i+1)(\mathcal{N}_i - v_i)v_j(\mathcal{N}_j - v_j + 1)}|\mathcal{N}_i, v_i+1, \mathcal{N}_j, v_j-1 >, \tag{46}$$

and using eq. (44) it is easy to verify that the operator

$$M_{ij} = -a_i^+ a_j - a_j^+ a_i - \frac{1}{2}[a_i, a_i^+][a_j, a_j^+] + \frac{1}{2}\mathcal{N}_i\mathcal{N}_j, \tag{47}$$

has the matrix elements given in eqs. (37)-(39).

Using eqs. (42), (45) and (47), the Hamiltonian of eq. (34) can then be written as

$$H = E_0' + \sum_{i=1}^{n} A_i'\{a_i, a_i^+\} + \sum_{i<j}^{n} A_{ij}'[a_i, a_i^+][a_j, a_j^+] + \sum_{i<j}^{n} \lambda_{ij}'(a_i^+ a_j + a_j^+ a_i), \tag{48}$$

where the constants E_0', A_i', A_{ij}', λ_{ij}' can be easily expressed in terms of the constants E_0, A_i, A_{ij}, λ_{ij} of eq. (34) and $\mathcal{N}_i$, $\mathcal{N}_j$.

A few comments are now in place:

i) The Hamiltonian of eq. (48) is fully equivalent to the one of Iachello and Oss (eq. (34)), when the generalized deformed bosons used in it are characterized by the structure function of eq. (29). However, the present formalism can be also used with generalized deformed bosons characterized by other structure functions related to vibrational molecular spectra. Thus the present formalism offers as a bonus a large number of exactly soluble models at no further computational cost.

ii) An exactly soluble model (as an example of comment i)) can be obtained by using the structure function

$$F(N) = [N + b\gamma], \tag{49}$$

where the brackets indicate the usual q-numbers of eq. (26). This structure function has been used by Chang and Yan for the description of vibrational molecular spectra in [5, 6]. If γ is allowed to be an appropriate function of the angular momentum J, a description of both rotational and vibrational molecular spectra is obtained [7, 8]. For $b = 0$ the usual q-deformed harmonic oscillator [2, 3] is obtained.

iii) Another example of exactly soluble model, according to i), is given by the structure function [11]

$$F(N) = [N + cN^2], \tag{50}$$

where again the brackets indicate the usual q-numbers of eq. (26). For $q = 1$ the brackets go away and this structure function is equivalent to the one characterizing the Morse potential (eq. (29)), used here. For $q \neq 1$ this structure function represents a q-deformation of the Morse potential, an approach alternative to the use of a potential described by an expansion in terms of Morse functions. It should be recalled at this point that improved descriptions of vibrational spectra of diatomic molecules have been obtained in terms of q-deformed anharmonic oscillators having the $U_q(2) \supset O_q(2)$ [9] and $SU_q(1,1)$ [10] symmetries. WKB equivalent potentials giving the same spectrum as these q-deformed anharmonic oscillators have been obtained in [13]. They are q-deformed versions of the modified Pöschl-Teller potential, which is connected to the Morse potential by a known transformation [15]. It is therefore clear that the need for q-deformed versions of the Morse potential occurs in these cases as well.

iv) In the case of polyatomic molecules having specific symmetries, such as the benzene [17, 18] or octahedral XY_6 molecules [16], the coefficients in eq. (48) get simplified, since the arguments used in refs. [16, 17, 18] are still valid. In the two examples just mentioned (benzene, octahedral molecules), all bonds are equivalent, so that $\mathcal{N}_i = \mathcal{N}$, $A'_i = A'$ for any i, $A'_{ij} = B$ for any i and j. For the off-diagonal couplings, described by the last term in eq. (48), different cases have to be considered. In the case of octahedral XY_6 molecules, for example, one has to distinguish between adjacent and opposite bonds, as in [16], while in the case of benzene nearest neighbour couplings, next to nearest neighbour couplings and opposite bond couplings, as in [17, 18], have to be considered.

v) The expression of the model of n coupled anharmonic oscillators of Iachello and Oss in terms of generalized deformed oscillators is also helpful in clarifying the connection between the present model and earlier models using coupled oscillators for the description of molecular vibrations. The usual Hamiltonian for the description of vibrational modes of polyatomic molecules reads [19]

$$H = \sum_i \omega_i (v_i + \frac{d_i}{2}) + \sum_i \sum_{k \geq i} x_{ik} (v_i + \frac{d_i}{2})(u_k + \frac{d_k}{2}), \tag{51}$$

where d_i, d_k are the degeneracies of the corresponding modes. It is clear that the first term of the Hamiltonian of eq. (51), as well as the parts of the second term with $i = k$, are equivalent to the second term in eq. (48), while the parts of the second term of eq. (51) with $k > i$ are included in the third term of eq. (48).

vi) Another example is provided by the Hamiltonian of Kellman [20]

$$H = (a_1^+ a_1 + a_2^+ a_2 + 1)(1 + \frac{1}{M}) - \frac{1}{M}(a_1^+ a_2 + a_2^+ a_1), \tag{52}$$

which is included in the first, second and fourth terms of eq. (48).

vii) Another Hamiltonian by Kellman [21]

$$H = \hbar\omega_0(n_1 + n_2 + 1) + \frac{\alpha}{2}((n_1 + \frac{1}{2})^2 + (n_2 + \frac{1}{2})^2)$$
$$+\alpha_{12}(n_1 + \frac{1}{2})(n_2 + \frac{1}{2}) + \frac{\beta}{2}(a_1^+ a_2 + a_2^+ a_1), \tag{53}$$

used for the description of vibrational spectra of ABA triatomics, is also a special case of eq. (48). In particular, the first two terms of the Hamiltonian of eq. (53) are contained in the second term of the Hamiltonian of eq. (48), while the third (fourth) term of eq. (53) corresponds to the third (fourth) term of eq. (48).

viii) Kellman has also used for the description of ABA triatomics the Hamiltonian [22]

$$H = \hbar\omega_s(n_s + \frac{1}{2}) + \hbar\omega_a(n_a + \frac{1}{2}) + \frac{\gamma_s}{2}(n_s + \frac{1}{2})^2 + \frac{\gamma_a}{2}(n_a + \frac{1}{2})^2$$
$$+\gamma_{sa}(n_s + \frac{1}{2})(n_a + \frac{1}{2}) + \delta(a_s^+ a_s^+ a_a a_a + a_a^+ a_a^+ a_s a_s), \tag{54}$$

of which the first four terms are equivalent to the second term of eq. (48), while its fifth term is contained in the third term of eq. (48). The last term of the Hamiltonian of eq. (54) is not contained in eq. (48). This term is suitable for reproducing the Darling-Dennison normal mode coupling [32]. In the case of the exactly soluble models expressed by the Hamiltonian of eq. (48), it is a trivial task to include such a term. The corresponding matrix elements are then

$$< \mathcal{N}_i, v_i + 2, \mathcal{N}_j, v_j - 2 | a_i^+ a_i^+ a_j a_j | \mathcal{N}_i, v_i, \mathcal{N}_j, v_j >$$
$$= \sqrt{F(v_i + 2)F(v_i + 1)F(v_j)F(v_j - 1)}. \tag{55}$$

For simple (not deformed) oscillators, for which $F(v_i) = v_i$, eq. (55) gives the Darling-Dennison result, while in the case of generalized deformed (anharmonic) oscillators the Darling-Dennison coupling is the lowest order term in an expansion using the anharmonicity constants as small parameters.

ix) A hamiltonian recently treated is [33]

$$H = a_0 I + b_0 \sum_{i=1}^{d} a_i^+ a_i + c_0 \sum_{i,j=1,(i<j)}^{d} (a_i^+ a_j + a_j^+ a_i)$$

$$+ d_0 \sum_{i=1}^{d} ((a_i^+)^2 + a_i^2) + c_0 \sum_{i,j=1,(i<j)}^{d} (a_i^+ a_j^+ + a_i a_j), \tag{56}$$

the second (third) term of which is contained in the second (fourth) term of the Hamiltonian of eq. (48), while its fourth and fifth terms are not included in eq. (48).

In conclusion, we have constructed in section 2 a generalized deformed oscillator giving the same spectrum as the Morse potential. Subsequently, in this section, the model of n coupled anharmonic oscillators of Iachello and Oss [16, 17, 18] was written in terms of such generalized oscillators. In addition to clarifying the relation of the model to existing models using coupled oscillators for the description of vibrational spectra of diatomic molecules [19, 20, 21, 22, 33], the present formalism allows for the construction of a large class of exactly soluble models with no extra computational effort. As an example, the way of including a term giving the Darling-Dennison coupling has been demonstrated.

Applications of some of the above mentioned exactly soluble models to vibrational spectra of specific polyatomic molecules should be carried out in order to check the relative significance of the various contributing terms.

The spectrum of the q-deformed harmonic oscillator can be also obtained from solving the q-deformed Schrödinger equation [34] for the usual harmonic oscillator potential. The q-deformed Schrödinger equation for the hydrogen atom has also been studied recently [35]. It will be interesting to construct the q-deformed Schrödinger equation for the Morse potential and check the changes inflicted by the q-deformation on the spectrum. It will also be of interest to construct the q-deformed Schrödinger equation for the modified Pöschl-Teller potential and check the relation between its eigenvalues and the spectrum of the q-deformed anharmonic oscillator with $\mathrm{SU}_q(1,1)$ symmetry of ref. [10], for which the WKB equivalent potential has been shown [13] to be a q-deformation of the usual modified Pōschl-Teller potential. The q-deformed version of the vibron model [23, 24] of molecular structure, as well as of the Interacting Boson Model of nuclear structure ([36, 37, 38], see [39, 40] for recent overviews) are also of interest, a step in this direction already taken in [41]. Work in these directions is in progress.

4. Models for vibrational and transitional nuclear spectra

One of the first applications of quantum algebras in physics came with the realization that rotational spectra of deformed nuclei, superdeformed nuclei and diatomic molecules can be accurately described by the quantum algebra $\mathrm{SU}_q(2)$ (see [4] for relevant references). The correspondence between the $\mathrm{SU}_q(2)$ expression and the Variable Moment of Inertia (VMI) model [42] has also been established [43]. It has been shown that in both cases the energy is described by a series in powers of $J(J+1)$, the deformation parameter q of the algebra been connected to the softness parameter of the VMI model. When the deformation parameter q is set equal to 1, the usual Lie algebra SU(2) is obtained.

It is not surprising that the applicability of the $\mathrm{SU}_q(2)$ formalism is limited to the rotational region (where the ratio $R_4 = E(4)/E(2)$ obtains values between 3.0 and 3.33), since it is based on a deformation of the rotation algebra. For describing nuclear spectra in the vibrational ($2.0 \leq R_4 \leq 2.4$) and transitional ($2.4 \leq R_4 \leq 3.0$) regions it is clear that an extension of the model is needed. In order to be guided towards such an extension, we briefly review the existing experience of other successful models:

i) In the rotational (SU(3)) limit [37] of the Interacting Boson Model (IBM) the spectrum is described by a $J(J+1)$ expression, while in the vibrational (U(5)) [36] and transitional (O(6)) [38] limits expressions of the form $J(J+c)$ with $c > 1$ appear. In the U(5) limit, in particular, the energy levels are given by

$$E(N, n_d, v, n_\Delta, J, M_J) = E_0 + \epsilon n_d + \alpha n_d(n_d+4) + \beta 2v(v+3) + \gamma 2J(J+1), \qquad (57)$$

where N is the total number of bosons, n_d is the number of d-bosons, v is the seniority, n_Δ is the "missing" quantum number in the reduction from O(5) to O(3), M_J is the third component of the angular momentum J, while E_0, ϵ, α, β, γ are free parameters. The ground state band, in particular, is characterized by quantum numbers $n_d = 0, 1, 2, \ldots, v = n_d$, $n_\Delta = 0$, $J = 2n_d$, so that the energy expression for it reads

$$E(J) = E_0 + \frac{\epsilon}{2}J + \frac{\alpha}{4}J(J+8) + \frac{\beta}{2}J(J+6) + 2\gamma J(J+1). \tag{58}$$

In the O(6) limit the energy is given by

$$E(N, \sigma, \tau, \nu_\Delta, J, M_J) = E_0 + \beta 2\tau(\tau+3) + \gamma 2J(J+1) + \eta 2\sigma(\sigma+4), \tag{59}$$

where σ is the quantum number characterizing the irreducible representations (irreps) of O(6), τ is the quantum number characterizing the irreps of O(5), ν_Δ is the missing quantum number in the reduction from O(5) to O(3), while E_0, β, γ, η are free parameters. The ground state band is characterized by the quantum numbers $\sigma = N$, $\tau = 0, 1, 2, \ldots$, $\nu_\Delta = 0$, $J = 2\tau$, so that the relevant energy expression takes the form

$$E(J) = E_0 + \frac{\beta}{2}J(J+6) + \gamma 2J(J+1) + \eta 2N(N+4). \tag{60}$$

The message from eqs (58) and (60) is that nuclear anharmonicities are described by expressions in which J and J^2 appear with different coefficients, and not with the same coefficient as in $J(J+1)$. The earliest introduction of this idea is in fact the Ejiri formula [44]

$$E(J) = kJ(J+1) + aJ, \tag{61}$$

which has been subsequently justified microscopically in [45].

ii) The two-parameter VMI model is known to continue giving good fits in the transitional and even in the vibrational region. In these regions, however, the accuracy of the model is substantially improved by adding a third parameter, which essentially allows for treating J and J^2 with a different coefficient [46, 47, 48].

In the usual VMI model [42] the levels of the ground state band are given by

$$E(J) = \frac{J(J+1)}{2\Theta(J)} + \frac{1}{2}C(\Theta(J) - \Theta_0)^2, \tag{62}$$

where C and Θ_0 are the two parameters of the model, the latter being the ground state moment of inertia. The moment of inertia for each J is determined from the variational condition

$$\frac{\partial E(J)}{\partial \Theta(J)}|_J = 0, \tag{63}$$

which leads to a cubic equation with only one real root. The energy can be written as an expansion in powers of $J(J+1)$ as [43]

$$E(J) = \frac{1}{2\Theta_0}(J(J+1) - \frac{\sigma}{2}(J(J+1))^2 + \sigma^2(J(J+1))^3 - 3\sigma^3(J(J+1))^4 + \ldots), \qquad (64)$$

where the softness parameter

$$\sigma = \frac{1}{2C\Theta_0^3} \qquad (65)$$

is serving as the small parameter of the expansion.

One of the (essentially equivalent) three-parameter extensions of the model, which give improved fits of vibrational and transitional spectra, is the generalized VMI (GVMI) model [46, 47], in which the energy levels are described by

$$E(J) = \frac{J + xJ(J-2)}{\Phi(J)} + \frac{1}{2}k(\Phi(J) - \Phi_0)^2, \qquad (66)$$

which can be easily rewritten in the form

$$E(J) = \frac{J(J+x')}{2\Phi'(J)} + \frac{1}{2}k'(\Phi'(J) - \Phi'_0)^2, \qquad (67)$$

where $x' = x^{-1} - 2$. It is clear that for $x = 1/3$ the GVMI reduces to the usual VMI, while for transitional and vibrational nuclei x obtains lower values [47], so that x' becomes greater than 1. The variational condition determining the moment of inertia still has the form of eq. (63), while the expansion of the energy turns out to be

$$E(J) = \frac{1}{2\Phi'_0}(J(J+x') - \frac{\sigma'}{2}(J(J+x'))^2 + (\sigma')^2(J(J+x'))^3 - 3(\sigma')^3(J(J+1))^4 + \ldots), \qquad (68)$$

where

$$\sigma' = \frac{1}{2k'(\Phi'_0)^3}. \qquad (69)$$

We remark that an expansion in terms of $J(J+x')$ is obtained, as compared to an expansion in terms of $J(J+1)$ in the case of the usual VMI. The physical content of the parameters is clear: the centrifugal stretching effect is accounted for by the softness parameter σ', as in the case of the usual VMI, while anharmonicities, important in the vibrational region, are introduced by $x' > 1$. Since centrifugal stretching and anharmonicities are two effects of different origins, it is reasonable to describe them by two different parameters.

In the case of the $SU_q(2)$ model the energy spectrum is given by the eigenvalues of the second order Casimir operator of the algebra, i.e.

$$E(J) = \frac{1}{2I}[j][j+1], \tag{70}$$

where q-numbers are defined as

$$[x] = \frac{q^x - q^{-x}}{q - q^{-1}}. \tag{71}$$

In the case of interest one has $q = e^{i\tau}$ (with τ real), so that

$$[x] = \frac{\sin(\tau x)}{\sin \tau}. \tag{72}$$

In this case the energy can be expanded as [43]

$$E(J) = \frac{1}{2I}\frac{1}{(j_0(\tau))^2}(j_0(\tau)J(J+1) - \tau j_1(\tau)(J(J+1))^2 + \frac{2}{3}\tau^2 j_2(\tau)(J(J+1))^3$$
$$-\frac{1}{3}\tau^3 j_3(\tau)(J(J+1))^4 + \frac{2}{15}\tau^4 j_4(\tau)(J(J+1))^5 - \ldots), \tag{73}$$

where $j_n(\tau)$ are the spherical Bessel functions of the first kind.

The evidence coming from the IBM and the generalized VMI model described above, suggests a model in which the spectrum is given by

$$E(J) = \frac{1}{2I}[J][J+c], \tag{74}$$

which contains 3 parameters: the moment of inertia I, the deformation parameter q and the new parameter c, which is expected to be 1 in the rotational limit and larger than 1 in the vibrational and transitional regions. This energy expression can be expanded as

$$E(J) = \frac{1}{2I}\frac{1}{(j_0(\tau))^2}(j_0(\tau)J(J+c) - \tau j_1(\tau)(J(J+c))^2 + \frac{2}{3}\tau^2 j_2(\tau)(J(J+c))^3$$
$$-\frac{1}{3}\tau^3 j_3(\tau)(J(J+c))^4 + \frac{2}{15}\tau^4 j_4(\tau)(J(J+c))^5 - \ldots), \tag{75}$$

which is similar to eq. (73) with $J(J+1)$ replaced by $J(J+c)$. It is expected that the deformation parameter τ, which plays the role of the small parameter in the expansion, as the softness parameter does in the case of the VMI, will describe the centrifugal stretching effect, while the parameter c will correspond to the anharmonicity effects. Numerical calculations involving fits to experimental data are in progress. A few comments are now in place:

i) It is worth remarking that eq. (74) coincides for $q = 1$ and c=integer=N with the eigenvalues of the Casimir operator of the algebra SO(N+2) in completely symmetric states [49]. In the rotational region one expects N=1, which corresponds to SO(3), while in the transitional and vibrational regions higher values of N are expected. The connection of the expression appearing in eq. (74) to the second order Casimir operator of a quantum algebra larger than SU$_q$(2) is an interesting question.

ii) The SU$_q$(2) symmetry is known to make specific predictions for the deviation of the behaviour of the B(E2) values from the rigid rotator model [50]. It will be interesting to connect the spectrum of eq. (74) to some deformed symmetry, at least for special values of c, and examine the implications of such a symmetry for the B(E2) values.

iii) It is worth noticing that an expansion in terms of $J(J+c)$ can also be obtained from a generalized oscillator [30] with a structure function

$$F(J) = [J(J+c)]_Q, \tag{76}$$

with

$$[x]_Q = \frac{Q^x - 1}{Q - 1} \tag{77}$$

and $Q = e^T$, with T real. This is similar to the oscillator successfully used in [11] for the description of vibrational spectra of diatomic molecules. It can also be considered as a deformation of the oscillator corresponding to the Morse potential, studied in section 2.

In conclusion, we have seen that an extension of the SU$_q$(2) model of rotational nuclear spectra is required, in order to make it applicable in the vibrational and transitional regions as well. The extension discussed above is in agreement with the Interacting Boson Model and the Generalized Variable Moment of Inertia model. In addition to the overall scale parameter, the model contains two parameters, one related to the centrifugal stretching and another related to nuclear anharmonicities. In the rotational region the model coincides with the usual SU$_q$(2) model, while in the transitional and vibrational regions the anharmonicity parameter plays a role. It will be interesting to check if the expression of eq. (74) can be connected to the second order Casimir operator of a quantum algebra larger than SU$_q$(2). The construction of a deformed version of the Interacting Boson Model ([36, 37, 38], see [39, 40] for recent overviews) is also of interest, since terms as the one appearing in eq. (74) are expected to occur there. Work in these directions is in progress.

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