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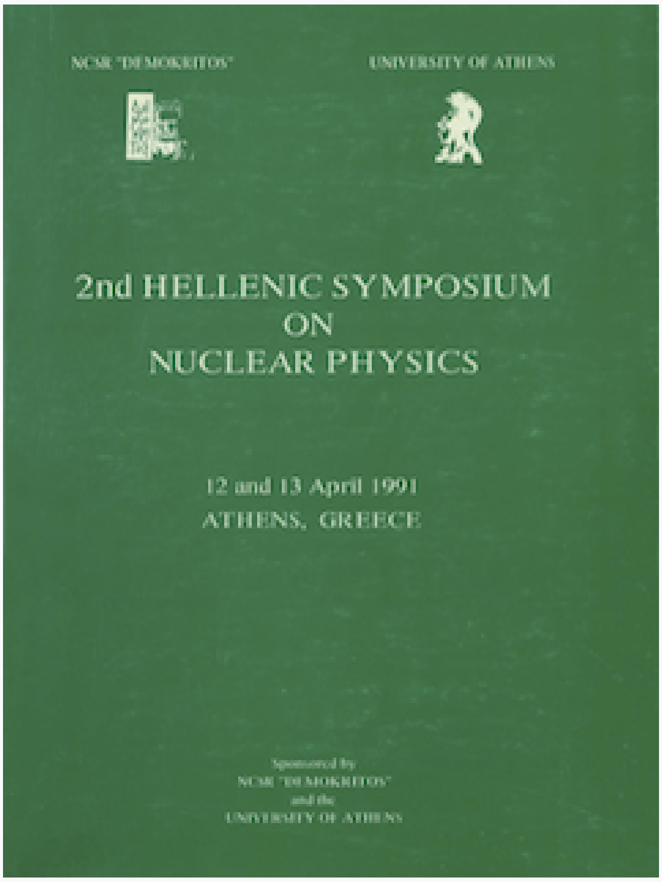

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QUANTUM ALGEBRAIC SYMMETRIES IN NUCLEAR AND MOLECULAR PHYSICS *

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Abstract

The first realizations of quantum algebraic symmetries in nuclear and molecular spectra are presented. Rotational spectra of even–even nuclei are described by the quantum algebra $SU_q(2)$. The two parameter formula given by the algebra is equivalent to an expansion in terms of powers of $j(j+1)$, similar to the expansion given by the Variable Moment of Inertia (VMI) model. The moment of inertia parameter in the two models, as well as the small parameter of the expansion, are found to have very similar numerical values. The same formalism is found to give very good results for superdeformed nuclear bands, which are closer to the classical SU(2) limit, as well as for rotational bands of diatomic molecules, in which a partial summation of the Dunham expansion for rotation–vibration spectra is achieved. Vibrational spectra of diatomic molecules can be described by the q-deformed anharmonic oscillator, having the symmetry $U_q(2)\supset O_q(2)$. An alternative description is obtained in terms of the quantum algebra $SU_q(1,1)$. In both cases the energy

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* Presented by Dennis Bonatsos

formula obtained is equivalent to an expansion in terms of powers of $(v+\frac{1}{2})$, where v is the vibrational quantum number, while in the classical SU(1,1) case only the first two powers appear. In all cases the improved description of the empirical data is obtained with q being a phase (and not a real number). Further applications of quantum algebraic symmetries in nuclei and molecules are discussed.

1. Introduction

Quantum algebras [1-5], or QUE (quantized universal enveloping) algebras, have been recently attracting much interest in physics [6-12]. They are generalizations of Lie algebras in which the associativity condition is a quantum Young-Baxter equation instead of the usual Jacobi identity [7]. These generalizations are called q-deformations of the corresponding Lie algebras, where q is the parameter characterizing the deformation. Mathematically they are Hopf algebras [13]. Sometimes they are referred to as quantum groups. In particular, the quantum algebra $SU_q(2)$ has been the subject of several investigations, since it is connected to the q-analogue of the quantum harmonic oscillator [6-12].

Here we give an account of realizations of quantum algebraic symmetries in nuclear and molecular physics. In section 2 the description of rotational spectra of deformed nuclei in terms of $SU_q(2)$ and its relation to the Variable Moment of Inertia (VMI) model is given. Superdeformed nuclear spectra are described by the same symmetry in section 3, while in section 4 this symmetry is used for the description of rotational spectra of diatomic molecules. Vibrational spectra of diatomic molecules are described in terms of the q-deformed anharmonic oscillator in section 5, while an alternative description of the same spectra in the framework of $SU_q(1,1)$ is given in section 6. Section 7 contains discussion of the present results and plans for further work.

2. $SU_q(2)$ description of rotational nuclear spectra and its relation to the Variable Moment of Inertia Model

It has been suggested [12] that spectra of rotational nuclei can be fitted very accurately using a Hamiltonian proportional to the second order Casimir operator of the quantum algebra $SU_q(2)$. It is therefore of great interest to understand the reasons of this success and their possible further consequences.

Here we examine the relation between the SU$_q$(2) expression for energies of ground state rotational bands to the usual expansion [14, 15] in terms of powers of $j(j+1)$ (where j is the angular momentum), as well as to the Variable Moment of Inertia (VMI) [16] formula, which is known [17, 18] to be equivalent to the Harris expansion [19] in terms of even powers of the angular velocity ω.

The generators J_+, J_0, J_- of the quantum algebra SU$_q$(2) [1-12] satisfy the commutation relations

$$[J_0, J_\pm] = \pm J_\pm, \tag{1}$$

$$[J_+, J_-] = [2J_0], \tag{2}$$

with $J_0^\dagger = J_0$, $(J_+)^\dagger = J_-$. The q-numbers are defined as

$$[x] = \frac{q^x - q^{-x}}{q - q^{-1}} = \frac{sinh(\tau x)}{sinh(\tau)}, \tag{3}$$

where $q = e^\tau$. In the limit $q \to 1$ ($\tau \to 0$) one clearly has $[x] \to x$, i.e. the q-numbers become usual numbers.

The irreducible representations D^j of SU$_q$(2) are determined by highest weight states with $j = 0, \frac{1}{2}, 1, \ldots$. The basic states $|j,m>$ $(-j \leq m \leq j)$ are connected with highest weight states $|j,j>$ as follows

$$|j,m> = \sqrt{\frac{[j+m]!}{[2j]![j-m]!}}(J_-)^{j-m}|j,j>, \tag{4}$$

with $J_+|j,j> = 0$ and $<j,j|j,j> = 1$. The second order Casimir operator of SU$_q$(2) is

$$C_2^q = J_-J_+ + [J_0][J_0+1], \tag{5}$$

for which one has

$$C_2^q|j,m> = [j][j+1]|j,m> . \tag{6}$$

A q-rotor is a system with Hamiltonian

$$H^q = \frac{1}{2I}C_2^q + E_0, \tag{7}$$

where I is the moment of inertia and E_0 is the bandhead energy (for ground state bands $E_0 = 0$). In the general case, i.e. with $q = e^{\tau}$, one has for the energy levels of the q-rotor

$$E_j = \frac{1}{2I}[j][j+1] + E_0 = \frac{1}{2I}\frac{sinh(\tau j) sinh(\tau(j+1))}{sinh^2(\tau)} + E_0. \tag{8}$$

In the special case of $\tau = i|\tau|$ one obtains

$$E_j = \frac{1}{2I}[j][j+1] + E_0 = \frac{1}{2I}\frac{sin(|\tau|j) sin(|\tau|(j+1))}{sin^2(|\tau|)} + E_0. \tag{9}$$

In [12] it has been found that good fits of rotational spectra of even–even rare earths and actinides are obtained with eq. (9). It is easy to check that eq. (8) fails in describing such spectra. In order to understand this difference, it is useful to make Taylor expansions of the quantities in the numerator of eq. (8) (eq. (9)) and collect together the terms containing the same powers of $j(j+1)$ (all other terms cancel out), finally summing up the coefficients of each power. In the first case the final result is

$$E_j = E_0 + \frac{1}{2I}\frac{1}{(\sqrt{\frac{\pi}{2\tau}}I_{1/2}(\tau))^2}(\sqrt{\frac{\pi}{2\tau}}I_{1/2}(\tau)j(j+1) + \tau\sqrt{\frac{\pi}{2\tau}}I_{3/2}(\tau)(j(j+1))^2$$

$$+\frac{2\tau^2}{3}\sqrt{\frac{\pi}{2\tau}}I_{5/2}(\tau)(j(j+1))^3 + \frac{\tau^3}{3}\sqrt{\frac{\pi}{2\tau}}I_{7/2}(\tau)(j(j+1))^4 + \dots \tag{10}$$

where $\sqrt{\frac{\pi}{2\tau}}I_{n+\frac{1}{2}}(\tau)$ are the modified spherical Bessel functions of the first kind [20].

In the second case (eq. (9)) following the same procedure one obtains

$$E_j = E_0 + \frac{1}{2I}\frac{1}{(j_0(|\tau|))^2}(j_0(|\tau|)j(j+1) - |\tau|j_1(|\tau|)(j(j+1))^2 + \frac{2}{3}|\tau|^2 j_2(|\tau|)(j(j+1))^3$$

$$-\frac{1}{3}|\tau|^3 j_3(|\tau|)(j(j+1))^4 + \frac{2}{15}|\tau|^4 j_4(|\tau|)(j(j+1))^5 - \dots), \tag{11}$$

where $j_n(\tau)$ are the spherical Bessel functions of the first kind [20].

Both results are of the form

$$E_j = E_0 + Aj(j+1) + B(j(j+1))^2 + C(j(j+1))^3 + D(j(j+1))^4 + \dots, \tag{12}$$

which is the expansion in terms of powers of $j(j+1)$ used for fitting experimental rotational spectra [15]. Empirically [15] it is known that the coefficients A, B, C, D, ... have alternating signs, starting with A positive. In addition, B is roughly three orders of magnitude smaller than A, C is about three orders of magnitude smaller than B, and D is also three orders of magnitude smaller than C [15].

It is interesting to check if the empirical characteristics of the coefficients A, B, C, D are present in the case of the expansions of eqs. (10), (11), especially for small values of τ or $|\tau|$. (Since we deal with rotational spectra, which are in first order approximation described by the usual algebra SU(2), we expect τ (or $|\tau|$) to be relatively small, i.e. the deviation of $\mathrm{SU}_q(2)$ from SU(2) to be small. This is in agreement to the findings of [12], where $|\tau|$ is found to be around 0.03.)

In (10) it is impossible to get alternating signs. The first term contains $\sqrt{\frac{\pi}{2\tau}}I_{1/2}(\tau)$, which is an even function of τ, positive for all values of τ [20]. The second term contains $\sqrt{\frac{\pi}{2\tau}}I_{3/2}(\tau)$, which is an odd function of τ, positive for positive τ [20]. However, the second term also contains τ, which has the same properties. Thus the second term is always positive. In the same way one can prove that all terms in (10) are positive, taking into account that $\sqrt{\frac{\pi}{2\tau}}I_{5/2}(\tau)$ is an even function of τ, $\sqrt{\frac{\pi}{2\tau}}I_{7/2}(\tau)$ is an odd function of τ [20], etc. We conclude that it is impossible to get alternating signs in eq. (10), i.e. this equation is inappropriate for describing nuclear rotational spectra.

In eq. (11), however, the situation is different. The first term contains $j_0(|\tau|)$, which is an even function of $|\tau|$, positive for small values of $|\tau|$ ($|\tau| < \pi$) [20]. The second term contains $j_1(|\tau|)$, which is an odd function of $|\tau|$, positive for small $|\tau|$ [20]. Thus the second term is negative, because of the minus sign appearing in front of it. In the same way it turns out that the third term is positive, the fourth term is negative, etc. The condition of alternating signs is thus fulfilled. In order to check the order of magnitude of the coefficients for small values of $|\tau|$, it is useful to expand the spherical Bessel functions appearing in (11) and keep only the lowest order term in each expansion. The result is

$$E_j = E_0 + \frac{1}{2I}(j(j+1) - \frac{|\tau|^2}{3}(j(j+1))^2 + \frac{2|\tau|^4}{45}(j(j+1))^3$$

$$-\frac{|\tau|^6}{315}(j(j+1))^4 + \frac{2|\tau|^8}{14175}(j(j+1))^5 - \ldots). \tag{13}$$

We remark that each term contains a factor $|\tau|^2$ more than the previous one. For $|\tau|$ in the area of 0.03, $|\tau|^2$ is of the order of 10^{-3}, as it should. We conclude therefore that eq. (11)

is suitable for fitting rotational spectra, since its coefficients have the same characteristics as the empirical coefficients of eq. (12). Examples of fits and parameter values are given in [21, 22]. In all cases the fits are of very good quality.

We now turn to the comparison of the expansion of eq. (11) to the Variable Moment of Inertia (VMI) [16] model. In this model the levels of the ground state band are given by

$$E_j = \frac{j(j+1)}{2\Theta(j)} + \frac{1}{2}C(\Theta(j) - \Theta_0)^2, \tag{14}$$

where C and Θ_0 are the two free 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

$$\frac{\partial E_j}{\partial \Theta(j)}|_j = 0, \tag{15}$$

which is equivalent to the cubic equation

$$\Theta(j)^3 - \Theta(j)^2\Theta_0 - \frac{j(j+1)}{2C} = 0. \tag{16}$$

This equation has only one real root, which can be written as

$$\Theta(j) = \sqrt[3]{\frac{j(j+1)}{4C} + \frac{\Theta_0^3}{27} + \sqrt{\frac{(j(j+1))^2}{16C^2} + \frac{\Theta_0^3 j(j+1)}{54C}}}$$

$$+\sqrt[3]{\frac{j(j+1)}{4C} + \frac{\Theta_0^3}{27} - \sqrt{\frac{(j(j+1))^2}{16C^2} + \frac{\Theta_0^3 j(j+1)}{54C}}} + \frac{\Theta_0}{3}. \tag{17}$$

Expanding the roots in eq. (17) and keeping together terms containing the same powers of $j(j+1)$ one obtains

$$\Theta(j) = \Theta_0\Big(1 + \frac{j(j+1)}{2C\Theta_0^3} - 2\frac{(j(j+1))^2}{(2C\Theta_0^3)^2} + 7\frac{(j(j+1))^3}{(2C\Theta_0^3)^3} - 30\frac{(j(j+1))^4}{(2C\Theta_0^3)^4} + \ldots\Big). \tag{18}$$

Using (16) in (14) one has

$$E_j = \frac{C}{2}(\Theta(j) - \Theta_0)(3\Theta(j) - \Theta_0). \tag{19}$$

Using (18) in (19) one obtains the following expansion for the energy

$$E_j = \frac{1}{2\Theta_0}(j(j+1) - \frac{1}{2}\frac{(j(j+1))^2}{2C\Theta_0^3} + \frac{(j(j+1))^3}{(2C\Theta_0^3)^2} - 3\frac{(j(j+1))^4}{(2C\Theta_0^3)^3} + \ldots) \tag{20}$$

It is known [16] that C and Θ_0 obtain positive values, while

$$\sigma = \frac{1}{2C\Theta_0^3}, \tag{21}$$

is the softness parameter, which for rotational nuclei is of the order of 10^{-3} [16]. Thus the coefficients of the expansion of eq. (20) have the proper signs and orders of magnitude.

Comparing eqs (11) and (20) we see that both expansions have the same form. The moment of inertia parameter I of (11) corresponds to the ground state moment of inertia Θ_0 of (20). The small parameter of the expansion is $|\tau|^2$ in the first case, while it is the softness parameter $1/(2C\Theta_0^3)$ in the second. However, the numerical coefficients in front of each power of $j(j+1)$ are not the same. In [21] a comparison is made between the parameters obtained from fitting the same spectra with eqs (11) and (20), the parameter values for the latter taken from [16]. The agreement between $1/(2I)$ and $1/(2\Theta_0)$ is very good, as it is the agreement between $|\tau|^2$ and σ as well. Therefore the known [16] smooth variation of Θ_0 and σ with the ratio $R_4 = E_4/E_2$ is expected to hold for the parameters I and $|\tau|^2$ as well. In fact, as seen in [21], larger R_4 leads to smaller $1/(2I)$ and smaller $|\tau|$ in both the rare earth and the actinide regions, as expected.

It is necessary for E_j to be an increasing function of j. In order to guarantee this in eq. (9) one must have

$$|\tau|(j+1) \leq \frac{\pi}{2}. \tag{22}$$

In the case of $|\tau| = 0.036$ (as in ^{232}U [21]), one finds $j \leq 42$, this limiting value being larger than the highest observed j in ground state bands in the actinide region [23]. Similarly, for $|\tau| = 0.046$ (as in ^{178}Hf [21]), one finds $j \leq 32$, this limiting value being again higher than the highest observed j in ground state bands in the rare earth region [23].

In conclusion, we have demonstrated that two different expansions of the second order Casimir operator of the quantum algebra SU$_q$(2) in terms of powers of $j(j+1)$ can be obtained, of which only one is suitable for the description of rotational ground state bands. This expansion is very similar to the one given by the Variable Moment of Inertia (VMI) model. The moment of inertia parameter, as well as the small parameter of the expansion, are very similar in both expansions. In addition to obtaining a two-parameter formula for ground state spectra alternative to the VMI one, we have shown that stretching effects can be taken into account by allowing the algebra to deviate from the usual SU(2) limit.

3. Description of superdeformed bands by the quantum algebra SU$_q$(2)

As we have seen in section 2, the quantum algebra SU$_q$(2) has been used for fitting the ground state bands of deformed rare earth and actinide nuclei [12, 21] with satisfactory results. On the other hand, the experimental discovery of superdeformation [24] (for relevant reviews see [25, 26]) has stirred considerable activity in the study of high spin states, the role of the pseudo–SU(3) symmetry in creating new magic numbers at high deformations [27], as well as the importance of the high N intruder orbitals [28, 29] for the properties of the superdeformed bands having been realized. It is therefore of great interest to examine to what extend the data for superdeformed bands can be described by the quantum algebra SU$_q$(2) and to point out the differences between such descriptions of rotational bands with normal and super deformations.

Eq. (9) has been used for fitting several superdeformed bands in the A=130 and A=150 regions, the results being reported in [22]. In addition, recently discovered superdeformed bands in the A=190 region have been fitted, also reported in [22]. For obtaining the fits an autoregularized iterational method of the Gauss–Newton type [30] has been used. In all cases the fits are of very good quality. In addition, the following comments apply:

i) In the case of the bands with normal deformation (section 2) the parameter $|\tau|$, which determines the spacing among the levels within a band, obtains values around 0.03. These values guarantee that the coefficients in the expansion of eq. (9) are small, following the pattern observed in ref. 15 (alternating signs, fall by approximately 3 orders of magnitude in successive coefficients). In addition, $|\tau|$ decreases with increasing collectivity (increasing $R_4 = E_4/E_2$ ratio, for example).

ii) In the case of superdeformed bands, $|\tau|$ obtains even smaller values, indicating that their symmetry is closer to the usual SU(2) symmetry. In particular, $|\tau|$ is about 0.01 in the A=130 and A=190 regions, which are assumed to correspond to axis ratios around 1.5:1 to 1.65:1 [24, 31], while it obtains even smaller values, around 0.004 in the A=150 region, which contains the best examples of superdeformed bands found so far, corresponding to an axis ratio close to 2:1 [24].

iii) In the case of the 2nd and 3rd superdeformed bands in ^{194}Hg, the levels of each of which are known [32] to lie midway of the levels of the other, almost identical parameter values are obtained.

Before concluding, it is appropriate to discuss a little further the physical motivation for using the quantum algebra SU$_q$(2) for the description of superdeformed bands. Three comments are then in place:

i) By defining, as usual,

$$J_+ = J_x + iJ_y, \qquad J_- = J_x - iJ_y, \qquad J_0 = J_z, \tag{23}$$

we can rewrite the SU$_q$(2) commutation relations (eqs (1) and (2)) in the form

$$[J_x, J_y] = \frac{i}{2}[2J_z], \qquad [J_y, J_z] = iJ_x, \qquad [J_z, J_x] = iJ_y, \tag{24}$$

which is the q-generalization of the SO(3) commutation relations, which are obtained from eq. (24) in the limit $q \to 1$. We remark that while in the classical SO(3) case the three commutation relations have exactly the same form, in the quantum case the first commutation relation in eq. (24) differs (in the right hand side) from the other two, thus indicating that the $z-$ direction is not any more equivalent to the $x-$ and $y-$ directions. Therefore it is not surprising that the SU$_q$(2) symmetry is more appropriate than the classical SU(2) symmetry for describing objects deformed in one of the 3 dimensions (like deformed and superdeformed nuclei).

ii) One could argue that the better description of deformed and superdeformed spectra obtained in the SU$_q$(2) case than in the SU(2) case is due to the extra parameter q (or, equivalently, τ) present in the first case. However, this is not an arbitrary additional parameter. As demonstrated in section 2 and ref. [21], the SU$_q$(2) expansion given in eq. (11) has the same form as the expansion of the VMI [16] formula in terms of $j(j+1)$. In addition, the τ^2 parameter of SU$_q$(2) corresponds [21] to the softness parameter σ of the VMI [16]. Therefore the parameter τ, which deforms the algebra, has a well-defined physical meaning.

iii) In the case of superdeformed bands, in particular, it has been demonstrated [33–35] that good fits can be obtained by using the Harris formalism [19]. (This fact has even been used for making spin assignments in the A=190 region [33–35].) However, the Harris formalism has been long known to be equivalent to the VMI approach [17, 18]. Since, as shown in [21], the $SU_q(2)$ formula is also equivalent to the VMI approach, it is not surprising that good fits of superdeformed spectra can be obtained in the $SU_q(2)$ framework as well.

In conclusion, we have demonstrated that superdeformed bands, as well as rotational bands with normal deformation, can be very accurately described in the framework of the quantum algebra $SU_q(2)$. Stretching effects are taken into account by allowing the algebra to deviate from the usual SU(2) limit. It has been demonstrated that this deviation is equivalent to an expansion in terms of powers of $j(j+1)$, summed up to all orders.

4. Description of rotational molecular spectra by the quantum algebra $SU_q(2)$

In section 2 it has been suggested that rotational bands in even–even nuclei can be described very accurately in terms of a Hamiltonian which is proportional to the second order Casimir operator of the quantum algebra $SU_q(2)$ [12, 21]. It is therefore of interest to examine if such a Hamiltonian can describe rotational spectra of molecules [36, 37] as well, and to understand the reasons of such a success and their further consequences.

Algebraic techniques have been already applied to the study of molecular rotation–vibration spectra [38–43], in analogy to a similar approach used for nuclear spectra ([44], for recent surveys see [45, 46]). The basic symmetry of diatomic molecules is U(4) [41, 42]. Of the various possible chains of subalgebras of U(4), the chains containing O(3) (which is isomorphic to SU(2)) are of interest, since angular momentum must be a good quantum number in this context.

In this section we examine if rotational spectra of diatomic molecules [36, 37] can be described in terms of the quantum algebra $SU_q(2)$. It is known [36, 37] that rotational molecular spectra are described by an expansion of the form

$$E_v(j) = B_v j(j+1) + D_v(j(j+1))^2 + H_v(j(j+1))^3 + J_v(j(j+1))^4 + \ldots, \tag{25}$$

where j is the angular momentum and v is the vibrational quantum number. More generally, rotation–vibration molecular spectra are described by the Dunham [47] expansion (for relevant reviews see [48, 49])

$$E(v,j) = \sum_{ik} Y_{ik}(v+\frac{1}{2})^i(j(j+1))^k, \tag{26}$$

where Y_{ik} are numerical coefficients. The first few terms of the Dunham expansion are known to occur from the solution [50] of the Schrödinger equation for the Morse potential [51]. By writing the Dunham expansion in the form

$$\begin{aligned}E(v.j) &= (Y_{00}+Y_{10}(v+\frac{1}{2})+Y_{20}(v+\frac{1}{2})^2+Y_{30}(v+\frac{1}{2})^3+\ldots)\\ &+j(j+1)(Y_{01}+Y_{11}(v+\frac{1}{2})+Y_{21}(v+\frac{1}{2})^2+Y_{31}(v+\frac{1}{2})^3+\ldots)\\ &+(j(j+1))^2(Y_{02}+Y_{12}(v+\frac{1}{2})+Y_{22}(v+\frac{1}{2})^2+Y_{32}(v+\frac{1}{2})^3+\ldots)\\ &+(j(j+1))^3(Y_{03}+Y_{13}(v+\frac{1}{2})+Y_{23}(v+\frac{1}{2})^2+Y_{33}(v+\frac{1}{2})^3+\ldots)+\ldots\end{aligned} \tag{27}$$

the relations between the coefficients B_v, D_v, H_v, ... and Y_{ik} become clear. Extensive tables of coefficients for several diatomic molecules can be found in [52]. In [53] we report the relevant coefficients for the HF, HCl, HBr molecules.

For the quantum algebraic description of rotational molecular spectra we use the algebra $SU_q(2)$. Both eqs. (10) and (11) are of the form shown in eq. (25), which is the expansion in terms of powers of $j(j+1)$ used for fitting experimental rotational spectra both in molecules [36] and nuclei [15]. Empirically [15, 36, 52] it is known that the coefficients B_v, D_v, H_v ... have alternating signs, starting with B_v positive. In addition, D_v is roughly 4–5 orders of magnitude smaller than B_v, and H_v is about 4–5 orders of magnitude smaller than D_v [36, 52].

It is interesting to check if the empirical characteristics of the coefficients B_v, D_v, H_v are present in the case of the expansions of eqs. (10), (11), especially for small values of τ or $|\tau|$. (Since we deal with rotational spectra, which are in first order approximation described by the usual algebra SU(2), we expect τ (or $|\tau|$) to be relatively small, i.e. the deviation of $SU_q(2)$ from SU(2) to be small. This is in agreement to the findings of [21] where $|\tau|$ is found to be around 0.03.)

As in section 2. alternating signs are gotten only in eq. (11) (and not in eq. (10)). In eq. (13) we remark that each term contains a factor $|\tau|^2$ more than the previous one. For $|\tau|$ in the area of 0.01, $|\tau|^2$ is of the order of 10^{-4}, as it should. We conclude therefore that eq. (11) (or eq. (9)) is suitable for fitting rotational spectra, since its coefficients have the same characteristics as the empirical coefficients of eq. (25). Examples of fits are reported in [53]. In all cases the fits are of very good quality. Since $|\tau|$ is small, it is clear from eq. (13) that $1/(2I)$ will be very close to $E_2(v)/6$. In addition, D_v/B_v should be approximately equal to $|\tau|^2/3$, i.e. $|\tau|$ should be close to $(3D_v/B_v)^{1/2}$. The values shown in [53] indicate that these approximate equalities hold very well. Even the small variation of the parameters between the $v = 0$ and $v = 1$ spectra of HCl are reproduced very well.

It is known that the Y_{ik} coefficients of the Dunham expansion are proportional to powers of the quantity (B_e/ω_e) [47, 48, 54], where B_e is the rotational constant in the equilibrium position and ω_e is the equilibrium vibrational constant [36]. A comparison of the expansion of eq. (13) to the expressions given in [47, 48, 54] shows that the role of the small parameter of the expansion played there by $(B_e/\omega_e)^2$ is played here by $|\tau|^2$. The situation resembles this in nuclear physics, where the correspondence between $|\tau|^2$ and the softness parameter σ of the Variable Moment of Inertia (VMI) Model [16] has been established [21].

From what we have already seen, it is clear that the usual expansion of rotational spectra in terms of $j(j+1)$ (eq. (25)) can be summed up through use of the $\mathrm{SU}_q(2)$ quantum algebra, as shown in eq. (9). In order to check the consequences of this finding for the Dunham expansion, we write eq. (26) as follows

$$\begin{aligned}E(v,j) = {}& (Y_{00} + Y_{01}j(j+1) + Y_{02}(j(j+1))^2 + Y_{03}(j(j+1))^3 + \ldots) + \\ & (v+\frac{1}{2})(Y_{10} + Y_{11}j(j+1) + Y_{12}(j(j+1))^2 + Y_{13}(j(j+1))^3 + \ldots) \\ & (v+\frac{1}{2})^2(Y_{20} + Y_{21}j(j+1) + Y_{22}(j(j+1))^2 + Y_{23}(j(j+1))^3 + \ldots) \\ & +(v+\frac{1}{2})^3(Y_{30} + Y_{31}j(j+1) + Y_{32}(j(j+1))^2 + Y_{33}(j(j+1))^3 + \ldots) + \ldots \qquad (28)\end{aligned}$$

Numerical values for the coefficients Y_{ik} for HF, HCl and HBr are reported in [53]. Data for other molecules can be found in [52]. We remark that Y_{01}, Y_{02}, Y_{03}, Y_{04} have alternating signs (starting with Y_{01} positive) and magnitudes falling by about 4 orders of magnitude from one to the next. Thus the terms in the first couple of parentheses in the rhs of eq. (28) look like the expansion in eq. (25) and can be summed up as eq. (9). A similar situation occurs for Y_{11}, Y_{12}, Y_{13}, ..., having as a result the summation of the terms in the second line of eq. (28), as well as for Y_{21}, Y_{22}, ..., resulting in the summation of the terms in the third line of eq. (28). We conclude that eq. (28) can be written as

$$E(v,j) = (Y_{00} + Y_0 \frac{sin(\tau_0 j) sin(\tau_0 (j+1))}{sin^2(\tau_0)}) + (Y_{10} + Y_1 \frac{sin(\tau_1 j) sin(\tau_1 (j+1))}{sin^2(\tau_1)})$$

$$+(Y_{20} + Y_2 \frac{sin(\tau_2 j) sin(\tau_2 (j+1))}{sin^2(\tau_2)}) + \dots \tag{29}$$

which implies that the Dunham expansion (eq. (26)) can be written in the form

$$E(v,j) = \sum_i (u + \frac{1}{2})^i (Y_{i0} + Y_i \frac{sin(\tau_i j) sin(\tau_i (j+1))}{sin^2(\tau_i)}), \tag{30}$$

where τ_i are real and positive, and the partial summation over powers of $j(j+1)$ has been carried out.

It is necessary for E_j to be an increasing function of j. In order to guarantee this in eq. (9) one must have

$$|\tau|(j+1) \leq \frac{\pi}{2}. \tag{31}$$

In the case of $|\tau| = 0.0174$ (as in HF [53]), one finds $j \leq 89$, while for $|\tau| = 0.0113$ (as in HBr [53]), one finds $j \leq 138$. These limiting values are higher than the highest observed j in these diatomic molecules [53].

In conclusion, we have demonstrated that two different expansions of the second order Casimir operator of the quantum algebra $SU_q(2)$ in terms of powers of $j(j+1)$ can be obtained, of which only one is suitable for the description of rotational molecular spectra. Rotational bands can be described in terms of two parameters, the moment of inertia I and the small parameter of the expansion, $|\tau|$, which is related to the Dunham coefficients. The Dunham series for rotation–vibration spectra of diatomic molecules can in this way be partially summed up.

5. Description of vibrational molecular spectra in terms of the q-anharmonic oscillator

In section 4 it has been demonstrated that a very accurate description of rotational molecular spectra can be obtained in terms of the quantum algebra $SU_q(2)$. It is therefore of interest to examine if an improved description of vibrational molecular spectra can also be obtained in a quantum algebraic framework.

Rotational–vibrational molecular spectra [36] are usually described in terms of the Dunham expansion (eq. (26)) [47, 48]. The first terms of the Dunham expansion are obtained from the exact solution [50] of the Schrödinger equation for the Morse potential [51]. They are also obtained in the O(4) limit of the U(4) algebraic model for diatomic molecular spectra [42], which has also been extended to triatomic molecules [43]. Ignoring angular momentum (i.e. ignoring the rotational bands built on each vibrational bandhead), the Dunham expansion takes the simplified form [48]

$$E(v) = \sum_i Y_{i0}(v + \frac{1}{2})^i, \tag{32}$$

i.e. an expansion in powers of $(v + \frac{1}{2})$.

In the algebraic framework, vibrational spectra of diatomic molecules have been described in terms of the anharmonic oscillator [55–58], using techniques similar to those used earlier in the algebraic approach to the Morse potential [59]. The relevant chain of subalgebras is U(2)⊃O(2). We briefly summarize here this approach, which we are going next to generalize. The generators of SU(2) take the form [57]

$$J_+ = a_1^+ a_2, \quad J_- = a_2^+ a_1, \quad J_0 = \frac{1}{2}(a_1^+ a_1 - a_2^+ a_2), \tag{33}$$

where a_1^+, a_1, a_2^+, a_2 satisfy usual boson commutation relations. The generators of SU(2) satisfy the commutation relations

$$[J_0, J_\pm] = \pm J_\pm, \tag{34}$$

$$[J_+, J_-] = 2J_0. \tag{35}$$

The basis takes the form

$$|v> = \frac{1}{\sqrt{(N-v)!v!}}(a_1^+)^v(a_2^+)^{N-v}|0>, \tag{36}$$

with $v = N_1$ and $N - v = N_2$. In the above N is the total number of bosons, N_1 (N_2) is the number of bosons with index 1 (index 2), and v is the vibrational quantum number.

The second order Casimir operator of the O(2) subalgebra takes the form [56]

$$C_2(O(2)) = 4J_0^2 = (a_1^+a_1 - a_2^+a_2)^2 = (N_1 - N_2)^2, \tag{37}$$

while the first order Casimir of U(2) is

$$C_1(U(2)) = N = N_1 + N_2 = a_1^+a_1 + a_2^+a_2, \tag{38}$$

i.e. the total number of bosons. (Recall that U(2) is obtained by supplying SU(2) with the additional generator N, which is the first order Casimir operator of U(2).) Finally, the Hamiltonian of the anharmonic oscillator takes the form [55, 58]

$$H = E_0 + A(C_1(U(2)))^2 - AC_2(O(2)) = 4(a_1^+a_1)(a_2^+a_2), \tag{39}$$

where A is a free parameter (the overall scale). The eigenvalues of this Hamiltonian in the above basis (eq. (36)) are

$$E(N,v) = E_0 + A4v(N-v). \tag{40}$$

This equation can be rewritten in the form

$$E(N,v) = -(2N+1) + 4(N+1)(v+\frac{1}{2}) - 4(v+\frac{1}{2})^2, \tag{41}$$

which shows that eq. (41) contains the first two powers of $(v+\frac{1}{2})$ contained in the Dunham expansion of eq. (32), the ratio of the coefficient of the first power over the coefficient of the second power (i.e. Y_{10}/Y_{20}) being $-(N+1)$.

In the case of the q-generalization of SU(2), called SU$_q$(2), the generators take the form [7]

$$J_+ = a_1^+a_2, \quad J_- = a_2^+a_1, \quad 2J_0 = N_1 - N_2, \tag{42}$$

where the operators a_i^+, a_i $(i = 1,2)$ satisfy the commutation relations

$$a_i a_i^+ - q^{-1} a_i^+ a_i = q^{N_i}, \quad i = 1,2. \tag{43}$$

In addition one has the relations

$$[N_i, a_i^+] = a_i^+, \quad [N_i, a_i] = -a_i, \quad i = 1,2, \tag{44}$$

as well as

$$a_i a_i^+ = [N_i + 1], \quad a_i^+ a_i = [N_i], \quad i = 1,2 \tag{45}$$

where q-numbers are defined as in section 2.

The generators of $\mathrm{SU}_q(2)$ satisfy the commutation relations given in section 2. The basis takes the form

$$|v> = \frac{1}{\sqrt{[v]![N-v]!}} (a_1^+)^v (a_2^+)^{N-v} |0>, \tag{46}$$

where $v = N_1$, $N - v = N_2$.

The first order Casimir operator of $\mathrm{U}_q(2)$ is [60]

$$C_1(U_q(2)) = [N] = [N_1 + N_2]. \tag{47}$$

As in the classical case mentioned above, $\mathrm{U}_q(2)$ is obtained by supplying $\mathrm{SU}_q(2)$ with this additional operator. By analogy to the classical case (eq. 39) the Hamiltonian takes the form

$$H = E_0 + A(C_1(U_q(2)))^2 - AC_2(O_q(2))$$

$$= E_0 + A[N_1 + N_2][N_1 + N_2] - A[N_1 - N_2][N_1 - N_2]. \tag{48}$$

Its eigenvalues in the basis of eq. (46) take, after a little of calculation, the form

$$E(N,v) = E_0 + A[2v][2N - 2v]. \tag{49}$$

This result goes to eq. (40) in the limit $q \rightarrow 1$. In the case $q = e^{\tau}$ eq. (49) takes the form

$$E(N,v) = E_0 + A\frac{sinh(2v\tau)sinh((2N-2v)\tau)}{sinh^2(\tau)}, \tag{50}$$

while in the case $q = e^{i\tau}$ one correspondingly has

$$E(N,v) = E_0 + A\frac{\sin(2v\tau)\sin((2N-2v)\tau)}{\sin^2(\tau)}. \tag{51}$$

It is instructive at this point to check how the last two equations compare to the Dunham expansion of eq. (32). In each case one can take the Taylor expansions of the functions appearing in the numerator of the right hand side, collect together terms containing the same power of $(v+\frac{1}{2})$, and finally sum up the coefficients of each power of $(v+\frac{1}{2})$. In the case of $q = e^{\tau}$ one obtains

$$\begin{aligned} E(N,v) = E_0 + A\frac{\tau^2}{\sinh^2(\tau)}[& -\frac{\sinh(\tau)\sinh(\tau(2N+1))}{\tau^2} + (v+\frac{1}{2})2\frac{\sinh(2\tau(N+1))}{\tau} \\ & -(v+\frac{1}{2})^2 4\cosh(2\tau(N+1)) + (v+\frac{1}{2})^3\frac{16}{3}\tau^2\frac{\sinh(2\tau(N+1))}{\tau} \\ & -(v+\frac{1}{2})^4\frac{16}{3}\tau^2\cosh(2\tau(N+1)) + (v+\frac{1}{2})^5\frac{64}{15}\tau^4\frac{\sinh(2\tau(N+1))}{\tau} \\ & -(v+\frac{1}{2})^6\frac{128}{45}\tau^4\cosh(2\tau(N+1)) + \ldots], \end{aligned} \tag{52}$$

while in the case of $q = e^{i\tau}$ one has

$$\begin{aligned} E(N,v) = E_0 + A\frac{\tau^2}{\sin^2(\tau)}[& -\frac{\sin(\tau)\sin(\tau(2N+1))}{\tau^2} + (v+\frac{1}{2})2\frac{\sin(2\tau(N+1))}{\tau} \\ & -(v+\frac{1}{2})^2 4\cos(2\tau(N+1)) + (v+\frac{1}{2})^3(-\frac{16}{3})\tau^2\frac{\sin(2\tau(N+1))}{\tau} \\ & -(v+\frac{1}{2})^4(-\frac{16}{3})\tau^2\cos(2\tau(N+1)) + (v+\frac{1}{2})^5\frac{64}{15}\tau^4\frac{\sin(2\tau(N+1))}{\tau} \\ & -(v+\frac{1}{2})^6\frac{128}{45}\tau^4\cos(2\tau(N+1)) + \ldots]. \end{aligned} \tag{53}$$

We remark that in both cases we obtain expressions resembling the Dunham expansion of eq. (32). In both cases in the limit $\tau \to 0$ one obtains the classical expression of eq. (41). For the ratio of the coefficient of the first power of $(v+\frac{1}{2})$ over the coefficient of the second power of $(v+\frac{1}{2})$ one has $-\tanh(2\tau(N+1))/(2\tau)$ in eq. (52), while one gets $-\tan(2\tau(N+1))/(2\tau)$ in eq. (53). In both cases in the limit $\tau \to 1$ one gets the classical value $-(N+1)$ [42]. However, it is clear that the extra parameter τ (or q), which is related to the deformation of the algebra. allows for this ratio to obtain values different from $-(N+1)$.

For a brief comparison to experimental data, we select the standard example of the $X^1\Sigma_g^+$ state of H_2 [61], which has been studied in the framework of the O(4) limit of the vibron model in [42]. (For a more sophisticated fitting, in the framework of the vibron model including higher order terms, see [62].) The potential curve of the $X^1\Sigma_g^+$ state of H_2, reported in [63], has been obtained [61] through use of the Rydberg–Klein–Rees (RKR) method [64–66]. For the $X^1\Sigma_g^+$ state of H_2 it is known that $v_{max} = 14$. Therefore, as in the case of [42], N can be either 28 or 29. We have selected the latter value. as in ref. [42]. (The former value also gives very similar results.) We have found [63] that an improved fit is obtained using eq. (53) (which corresponds to $q = e^{i\tau}$), while eq. (52) (which corresponds to $q = e^{\tau}$) does not improve the fit. The situation is the same as in the case of rotational spectra of diatomic molecules [53] or deformed nuclei [12, 21]. In these cases it has also been found that the choice of q being a phase ($q = e^{i\tau}$) was the one giving improved results. The results of the fit are given in [63]. A clear improvement is seen.

The potential corresponding to the Dunham expansion is known to have the form [47, 48]

$$V(x) = a_0 x^2 (1 + \sum_j a_j x^j). \tag{54}$$

It will be interesting to examine the consequences of the q-deformation on the potential. In this direction, the known relations [47, 48, 54] between the Y_{ik} coefficients of eq. (26) and the coefficients a_j of eq. (54) could be used.

In conclusion, we have shown that quantum algebras can be used for the description of vibrational spectra of diatomic molecules, using techniques similar to those used for the description of rotational spectra of diatomic molecules. While the Hamiltonian of the anharmonic oscillator, having the symmetry $U(2) \supset O(2)$, corresponds to the first two terms of the vibrational Dunham expansion, the Hamiltonian of the q-deformed anharmonic oscillator, having the generalized symmetry $U_q(2) \supset O_q(2)$, corresponds to all terms of the vibrational Dunham expansion, summed up in closed form. It also corresponds to partially summing up the more general Dunham expansion of eq. (26). A similar partial summation of the Dunham series, concerning the rotational quantum number, has been obtained in section 4 and ref. [53] using a q-deformed rotor having $SU_q(2)$ symmetry. It is then plausible that one could fully sum up the Dunham series by considering a more general quantum algebra having the vibrational quantum U(2) and the rotational quantum SU(2) (each of them having different value of q) as subalgebras.

6. $SU_q(1,1)$ description of vibrational molecular spectra

The Morse potential [51], which offers a widely accepted description of vibrational spectra of diatomic molecules [36], has been known to have the symmetry SU(1,1) [39, 40, 59, 67–70]. Vibrational spectra are then described by a Hamiltonian which is proportional to the second order Casimir operator of SU(1,1). In section 4 we have seen that an improved description of rotational spectra of diatomic molecules can be given by generalizing the classical SU(2) algebra into the quantum $SU_q(2)$ one. It is therefore of interest to check the consequences and the physical content of generalizing SU(1,1) into the quantum algebra $SU_q(1,1)$, which is already known [60, 71].

In the classical case [70] the SO(2,1) generators satisfy the commutation relations

$$[K_1, K_2] = -iK_3, \qquad [K_2, K_3] = iK_1, \qquad [K_3, K_1] = iK_2. \tag{55}$$

Defining

$$K_+ = K_1 + iK_2, \qquad K_- = K_1 - iK_2, \qquad K_3 = K_z, \tag{56}$$

one obtains the SU(1,1) commutation relations

$$[K_z, K_\pm] = \pm K_\pm, \qquad [K_+, K_-] = -2K_z. \tag{57}$$

The generators of SU(1,1) accept the following boson representation [67]

$$K_+ = a_1^+ a_2^+, \qquad K_- = a_1 a_2, \qquad K_z = \frac{1}{2}(a_1^+ a_1 + a_2^+ a_2 + 1), \tag{58}$$

where a_1^+, a_1, a_2^+, a_2 satisfy usual boson commutation relations.

The second order Casimir operator of SO(2,1) is [70]

$$C_2[SO(2,1)] = -(K_1^2 + K_2^2 - K_3^2). \tag{59}$$

If N is the number of excitation quanta given to the system (which is equal to the total number of bosons in the case of the boson representation) and v is the vibrational quantum number, the eigenvalues of the Casimir operator are given in

$$C_2[SO(2,1)]|N\omega> = \frac{1}{4}\omega(\omega+2)|N\omega>, \tag{60}$$

where the quantum number ω is given by

$$v = \frac{1}{2}(N-\omega). \tag{61}$$

N is related to the maximum number of vibrational states by

$$N = 2v_{max} \quad or \quad N = 2v_{max}+1. \tag{62}$$

The vibrational spectrum is given by

$$E(N,\omega) = E_0 - A < C_2[SO(2,1)] > = E_0 - \frac{A}{4}\omega(\omega+2), \tag{63}$$

where by $<>$ we denote the eigenvalue of the enclosed operator. Using (61) this can be rewritten as

$$E(N,v) = E_0 - A\frac{N^2-1}{4} + AN(v+\frac{1}{2}) - A(v+\frac{1}{2})^2. \tag{64}$$

Rotational–vibrational molecular spectra are usually described in terms of the Dunham expansion (eq. (26)) [47. 48]. Ignoring rotation (i.e. ignoring the rotational bands built on the vibrational bandheads) one obtains the vibrational spectrum given in eq. (32). We remark that eq. (64) corresponds to the first two nonvanishing powers of $(v+\frac{1}{2})$ contained in the Dunham expansion. The same result is obtained by solving [50] the Schrödinger equation for the Morse potential [51]. It is also obtained in the O(4) limit of the vibron model [42] for diatomic molecules, which has been extended to triatomic molecules [43, 56] and to higher order terms [62]. The ratio Y_{20}/Y_{10} (the anharmonicity constant [59]) is in the present case proportional to $1/N$, a result similar to the one obtained in the vibron model [42].

In the quantum case, the generators of SU$_q$(1,1) satisfy the commutation relations [60, 71]

$$[K_0, K_\pm] = \pm K_\pm, \qquad [K_+, K_-] = -[2K_0], \tag{65}$$

where q-numbers are defined as in section 2.

The generators of SU$_q$(1,1) accept the following boson representation [60, 71]

$$K_+ = a_1^+ a_2^+, \qquad K_- = a_1 a_2, \qquad K_0 = \frac{1}{2}(N_1 + N_2 + 1), \tag{66}$$

where the bosons a_i^+, a_i ($i = 1, 2$) satisfy eqs (43) and (44).

The second order Casimir operator of SU$_q$(1,1) is [60]

$$C_2[SU_q(1,1)] = [K_0][K_0 - 1] - K_+K_- = [K_0][K_0 + 1] - K_-K_+. \tag{67}$$

Its eigenvalues are given in [60]

$$C_2[SU_q(1,1)]|\kappa\mu >= [\kappa][\kappa - 1]|\kappa\mu >, \tag{68}$$

where

$$\kappa = \frac{1 + |n_1 - n_2|}{2}, \quad \mu = \frac{1 + n_1 + n_2}{2}, \tag{69}$$

since the basis has the form $|\kappa\mu >= |n_1 > |n_2 >$, with [60]

$$|n_i >= \frac{1}{\sqrt{[n_i]!}}(a_i^+)^{n_i}|0 > . \tag{70}$$

The vibrational spectrum is given by

$$H = E_0 - AC_2[SU_q(1,1)]. \tag{71}$$

Using the relation $|n_1 - n_2| = \omega + 1$ one obtains

$$E(N, \omega) = E_0 - A\left[\frac{\omega}{2}\right]\left[\frac{\omega + 2}{2}\right], \tag{72}$$

which in the limit $q \rightarrow 1$ goes to eq. (63). Using further eq. (61) one has

$$E(N, v) = E_0 - A\left[v - \frac{N}{2}\right]\left[v + 1 - \frac{N}{2}\right], \tag{73}$$

which is the q-generalization of eq. (64).

It is interesting to check how eq. (73) is related to eq. (64) and to the Dunham expansion (eq. (32)). This can be done by replacing the q-numbers in eq. (73) by their equals from eq. (3), subsequently taking the Taylor expansions of the hyperbolic (or trigonometric) functions, collecting together terms containing the same power of $(v+\frac{1}{2})$, and finally summing up the coefficients of each power of $(v+\frac{1}{2})$. In the case of real q the final result is

$$E(N,v)=E_0+\frac{A}{\sinh(\tau)^2}[-\frac{1}{2}(\cosh(\tau)-\cosh(\tau N))+\tau\sinh(\tau N)(v+\frac{1}{2})$$

$$-\tau^2\cosh(\tau N)(v+\frac{1}{2})^2+\frac{2}{3}\tau^3\sinh(\tau N)(v+\frac{1}{2})^3-\frac{1}{3}\tau^4\cosh(\tau N)(v+\frac{1}{2})^4$$

$$+\frac{2}{15}\tau^5\sinh(\tau N)(v+\frac{1}{2})^5-\frac{2}{45}\tau^6\cosh(\tau N)(v+\frac{1}{2})^6+\ldots], \tag{74}$$

while in the case of q being a phase the final result is

$$E(N,v)=E_0+\frac{A}{\sin(\tau)^2}[-\frac{1}{2}(\cos(\tau)-\cos(\tau N))+\tau\sin(\tau N)(v+\frac{1}{2})$$

$$-\tau^2\cos(\tau N)(v+\frac{1}{2})^2+(-\frac{2}{3})\tau^3\sin(\tau N)(v+\frac{1}{2})^3-(-\frac{1}{3})\tau^4\cos(\tau N)(v+\frac{1}{2})^4$$

$$+\frac{2}{15}\tau^5\sin(\tau N)(v+\frac{1}{2})^5-\frac{2}{45}\tau^6\cos(\tau N)(v+\frac{1}{2})^6+\ldots]. \tag{75}$$

The following remarks can now be made:

i) Both eq. (74) and eq. (75) reduce to eq. (64) in the limit $q\rightarrow 1$ $(\tau\rightarrow 0)$.

ii) While eq. (64) contains only the first two nonvanishing powers of $(v+\frac{1}{2})$, eqs (74) and (75) contain all possible powers. Thus eqs (74) and (75) correspond to the full Dunham expansion (eq. (32)). However, while the Y_{ik} coefficients in eq. (32) are not related to each other, their counterparts in eqs (74) (or eq. (75)) are interrelated, since they all depend on τ and N.

iii) The anharmonicity constant (i.e. the ratio Y_{20}/Y_{10}), which in the classical case (eq. (64)) is fixed to $-1/N$, it is here $-\tau/\sinh(\tau N)$ (in eq. (74)) or $-\tau/\sin(\tau N)$ (in eq. (75)). Therefore the anharmonicity constant is not fixed by N (or, equivalently through eq. (62), by v_{max}). This extra freedom is useful when one attempts to fit experimental data, as it will be demonstrated below.

For the briefest possible comparison to experimental data we consider the case of H_2 in its $X^1\Sigma_g^+$ state, which has been considered in the case of the anharmonic oscillator (section

5) as well. We first fitted the data using the classical eq. (64). When attempting to use eq. (74) one is driven to failure, while eq. (75) gives a result much better than eq. (64), as it can be seen in [72], where the results are reported. Thus the data indicate that q should be a phase, and not a real number. This conclusion is the same as the one drawn from the comparison of the q-rotor (having the symmetry $SU_q(2)$) to the rotational spectra of deformed [12, 21] and superdeformed [22] nuclei, as well as to the rotational spectra of diatomic molecules [53]. It should also be pointed out that the parameter τ remains small in all cases.

In conclusion, we have shown that the quantum algebra $SU_q(1,1)$ can be used for the description of vibrational spectra of diatomic molecules, in the same way as the quantum algebra $SU_q(2)$ can be used for the description of rotational spectra of molecules [53] and nuclei [12, 21, 22]. The second order Casimir operator of $SU_q(1,1)$ corresponds to a special form of the Dunham expansion containing all powers of $(v+\frac{1}{2})$, while in the classical case of SU(1,1) only the first two nonvanishing powers of $(v+\frac{1}{2})$ are obtained [39, 40, 59, 67–70].

In the classical case the relation between the second order Casimir operator of SO(2,1) and the eigenvalues of the Morse potential is known [70]. It is interesting to find the relation between the second order Casimir operator of $SU_q(1,1)$ and the eigenvalues of the Morse potential in the quantum case. For the latter, the q-Schrödinger equation [73] for the Morse potential should be solved. In addition, it is worth evaluating dissociation rates for the Morse potential in the quantum case, by generalizing the procedure outlined in [74].

7. Discussion

We have demonstrated that quantum algebras can give improved descriptions of rotational spectra of deformed and superdeformed nuclei, as well as of rotational and vibrational spectra of diatomic molecules. These successes call for further investigations, some of which are listed here:

i) It is interesting to check what forms of classical potentials give the same spectra as the q-harmonic oscillator, the q-rotor and the q-anharmonic oscillator. Progress in this direction is reported in the talk of Costas Daskaloyannis [75].

ii) Can the quantum algebra $SU_q(3)$ be successfully used for the description of rotational nuclear spectra?

iii) Can the q-generalizations of the O(4) and U(3) limits of the vibron model [42] (which has U(4) symmetry) give improved descriptions of molecular spectra?

iv) Can the q-generalizations of the U(5), SU(3) and O(6) limits of the Interacting Boson Model (IBM) [44] (which has U(6) symmetry) give improved descriptions of nuclear spectra?

v) The q-generalized Schrödinger equation has been recently solved for the harmonic oscillator, giving the q-deformed harmonic oscillator spectrum [73]. It will be interesting to see what spectrum is obtained by solving the q-Schrödinger equation for the Morse potential.

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