Molecular Spectra from Rotationally Invariant Hamiltonians
Based on the Quantum Algebra $su_q(2)$
and Irreducible Tensor Operators under $su_q(2)$

DENNIS BONATSOS#1, B. A. KOTSOS*2, P. P. RAYCHEV†3, P. A. TERZIEV†4

# Institute of Nuclear Physics, N.C.S.R. “Demokritos”,
GR-15310 Aghia Paraskevi, Attiki, Greece
* Department of Electronics, Technological Education Institute,
GR-35100 Lamia, Greece
† Institute for Nuclear Research and Nuclear Energy, Bulgarian Academy of Sciences,
72 Tzarigrad Road, BG-1784 Sofia, Bulgaria

ABSTRACT

The rotational invariance under the usual physical angular momentum of the $su_q(2)$ Hamiltonian for the description of rotational molecular spectra is explicitly proved and a connection of this Hamiltonian to the formalism of Amal’sky is provided. In addition, a new Hamiltonian for rotational spectra is introduced, based on the construction of irreducible tensor operators (ITOs) under $su_q(2)$ and use of $q$-deformed tensor products and $q$-deformed Clebsch–Gordan coefficients. The rotational invariance of this $su_q(2)$ ITO Hamiltonian under the usual physical angular momentum is explicitly proved and a simple closed expression for its energy spectrum (the “hyperbolic tangent formula”) is introduced. Numerical tests against an experimental rotational band of HF are provided.

1 Introduction

Quantum algebras [1, 2, 3] have started finding applications in the description of symmetries of physical systems over the last years [4], triggered by the introduction of the $q$-deformed harmonic oscillator [5, 6, 7]. In one of the earliest attempts, a Hamiltonian proportional to the second order Casimir operator of $su_q(2)$ has been used for the description of rotational molecular [8] and nuclear spectra [9] and its relation to the Variable Moment of Inertia Model [10] has been clarified.

However, several open problems remained:

a) Is the $su_q(2)$ Hamiltonian invariant under the usual $su(2)$ Lie algebra, i.e. under usual angular momentum, or it breaks spherical symmetry and/or the isotropy of space?
b) How does the physical angular momentum appear in the framework of $su_q(2)$? Is there any relation between the generators of $su_q(2)$ and the usual physical angular momentum operators?

---

1 e-mail: bonat@inp.demokritos.gr
2 e-mail: bkotsos@teilam.gr
3 e-mail: raychev@phys.uni-sofia.bg, raychev@inrne.bas.bg
4 e-mail: terziev@inrne.bas.bg
c) How can one add angular momenta in the su\(_q(2)\) framework? In other words, how does angular momentum conservation work in the su\(_q(2)\) framework?

Answers to these questions are provided in the present paper, along with connections of the su\(_q(2)\) model to other formalisms.

In Section 2 a brief description of the \(q\)-deformed harmonic oscillator is given, while in Section 3 the connection between the \(q\)-deformed harmonic oscillator and the usual harmonic oscillator is established through the use of \(q\)-deforming boson functionals, a tool which will be needed in the framework of su\(_q(2)\) as well. The su\(_q(2)\) formalism is briefly described in Section 4, while in Section 5 a representation of su\(_q(2)\) in terms of \(q\)-deformed boson operators is given. Based on this boson representation the connection between the su\(_q(2)\) quantum algebra and the usual su(2) Lie algebra is established in Section 6 and used in Section 7 for proving explicitly that the su\(_q(2)\) Hamiltonian does commute with the generators of su(2), i.e. with the generators of usual physical angular momentum. Therefore the su\(_q(2)\) Hamiltonian does not violate the isotropy of space and does not destroy spherical symmetry. The su\(_q(2)\) basis turns out to be identical to the usual su(2) basis in the boson representation under discussion. In addition, it turns out that the angular momentum quantum numbers appearing in the description of the su\(_q(2)\) states are exactly the same as the ones appearing in the states of su(2), establishing an one-to-one correspondence between the two sets of states (in the generic case in which the deformation parameter \(q\) is not a root of unity).

Taking advantage of the results of Section 7, we write in Section 8 the eigenvalues of the su\(_q(2)\) Hamiltonian as an exact power series in \(l(l + 1)\) (where \(l\) is the usual physical angular momentum). An approximation to this expansion, studied in Section 9, leads to a closed energy formula for rotational spectra introduced by Amal’sky \[11\].

We then turn in Section 10 into the study of irreducible tensor operators under su\(_q(2)\) \[12\] \[13\], constructing the irreducible tensor operator of rank one corresponding to the su\(_q(2)\) generators. We also define tensor products in the su\(_q(2)\) framework and construct the scalar square of the angular momentum operator, a task requiring the use of \(q\)-deformed Clebsch–Gordan coefficients \[12\]. In addition to exhibiting explicitly how addition of angular momenta works in the su\(_q(2)\) framework, this exercise leads to a Hamiltonian built out of the components of the above mentioned irreducible tensor operator (ITO), which can also be applied to the description of rotational spectra. We are going to refer to this Hamiltonian as the su\(_q(2)\) ITO Hamiltonian.

The fact that the su\(_q(2)\) ITO Hamiltonian does commute with the generators of the usual su(2) algebra is shown explicitly in Section 11. Based on the results of Section 11, we express in Section 12 the eigenvalues of the su\(_q(2)\) ITO Hamiltonian as an exact power series in \(l(l + 1)\), where \(l\) is the usual physical angular momentum. An approximation to this series, studied in Section 13, leads to a simple closed formula for the spectrum (the “hyperbolic tangent formula”).

Finally in Section 14 all the exact and closed approximate energy formulae obtained above are compared to the experimental spectrum of a rotational band of HF, which exhibits sizeable deviations from pure rotational behavior, as well as to the results provided by the usual rotational expansion and by the Holmberg–Lipas formula \[14\], which is probably the best two-parameter formula for the description of rotational nuclear spectra \[15\]. A discussion of the present results and plans for future work are given in Section 15.

2 The \(q\)-Deformed Harmonic Oscillator

The \(q\)-deformed harmonic oscillator \[3\] \[6\] \[7\] is defined by means of the operators \(a^\dagger\) and \(a\), which are referred to as \(q\)-deformed boson creation and annihilation operators, together with
the $q$-deformed number operator $N$. These operators close the $q$-deformed Heisenberg–Weyl algebra

\[ [a, a^\dagger]_q \equiv aa^\dagger - qa^\dagger a = q^{-N}, \quad [a, a^\dagger]_{q^{-1}} \equiv aa^\dagger - q^{-1}a^\dagger a = q^N, \]
\[ [N, a^\dagger] = a^\dagger, \quad [N, a] = -a. \tag{2} \]

From Eq. (1) one can easily see that the products of operators $a$ and $a^\dagger$ are equal to

\[ a^\dagger a = [N], \quad aa^\dagger = [N + 1], \tag{3} \]

where the square brackets denote $q$-operators, defined as

\[ [X] = \frac{q^X - q^{-X}}{q - q^{-1}}. \tag{4} \]

$q$-numbers are also defined in the same way. For the deformation parameter $q$ two different cases occur:

a) If $q$ is real, one can write $q = e^\tau$, where $\tau$ is real. Then one immediately sees that

\[ [X] = \frac{\sinh \tau X}{\sinh \tau}. \tag{5} \]

b) If $q$ is a phase factor (but not a root of unity, in which case one has $q^n = 1$, with $n \in \mathbb{N}$), one can write $q = e^{i\tau}$, where $\tau$ is real. Then one has

\[ [X] = \frac{\sin \tau X}{\sin \tau}. \tag{6} \]

In both cases one has

\[ [X] \to X \quad \text{as} \quad q \to 1. \tag{7} \]

There exists a state $|0\rangle_q$ (called the $q$-vacuum) with the properties

\[ a|0\rangle_q = 0, \quad N|0\rangle_q = 0. \tag{8} \]

Acting on this state with the operator $a^\dagger$ repeatedly, one can build up the states

\[ |n\rangle_q = \frac{(a^\dagger)^n}{\sqrt{|n|!}}|0\rangle_q, \tag{9} \]

where the quantity

\[ |n|! = [n][n - 1] \ldots [1] \tag{10} \]

is the $q$-factorial.

The states (9) form an orthonormal basis

\[ q\langle n|m\rangle_q = \delta_{nm}; \tag{11} \]

and are eigenvectors of the $q$-deformed number operator

\[ N|n\rangle_q = n|n\rangle_q. \tag{12} \]

From the last equation it is clear why the states of Eq. (9) are interpreted as states containing $n$ $q$-deformed bosons.
3 Connection of the $q$-Deformed Oscillator to the Usual Harmonic Oscillator

In the limit $q \to 1$ (or $\tau \to 0$) Eq. (11) is reduced into the commutation relation for usual boson creation and annihilation operators, for which the symbols $b^\dagger$ and $b$ will be used

$$[b, b^\dagger] = 1. \quad (13)$$

Furthermore, in the limit $q \to 1$ Eq. (2) is reduced into the form

$$[B, b^\dagger] = b^\dagger, \quad [B, b] = -b, \quad (14)$$

where by $B$ we denote the number operator, for which the following analogues of Eq. (3) are valid

$$b^\dagger b = B, \quad bb^\dagger = B + 1. \quad (15)$$

In analogy with Eq. (8) one can introduce the vacuum state $|0\rangle_c$ (the “classical” vacuum) with the properties

$$b|0\rangle_c = 0, \quad B|0\rangle_c = 0. \quad (16)$$

Then one can build up the states

$$|n\rangle_c = \frac{(b^\dagger)^n}{\sqrt{n!}} |0\rangle_c, \quad (17)$$

which form an orthonormal basis

$$c\langle n|m \rangle_c = \delta_{nm}, \quad (18)$$

and are eigenstates of number operator $B$, i.e.

$$B|n\rangle_c = n|n\rangle_c. \quad (19)$$

From the last equation it is clear that the states of Eq. (17) are states which contain $n$ bosons. The analogy between the “standard” and the $q$-deformed case is clear.

There is however a closer relation between the operators $a^\dagger (a)$ and $b^\dagger (b)$. In the space determined by the vectors of Eq. (17) one can define the operators

$$a = b \sqrt{\frac{B}{B}} \quad \text{and} \quad a^\dagger = \sqrt{\frac{B}{B}} b^\dagger. \quad (20)$$

It should be noticed that the definitions of Eq. (20) are meaningful only in the space of vectors $|n\rangle_c$, i.e. when the operators $a^\dagger$ and $a$ act on the vectors of Eq. (17). As a consequence the operator $B$, which appears in the denominator of Eq. (20), can be replaced by the number $n$ only when $a^\dagger$ or $a$ act on $|n\rangle_c$.

One can now calculate the bilinear products of $a^\dagger$ and $a$

$$a^\dagger a = \sqrt{\frac{B}{B}} \frac{b^\dagger b}{B} \sqrt{\frac{B}{B}} = [B], \quad (21)$$
In the derivation of the last equation the fact that for an arbitrary function \( f(B) \) one has

\[
b^\dagger f(B) = f(B - 1)b^\dagger, \quad \text{and} \quad bf(B) = f(B + 1)b,
\]

as well as Eq. (15) have been taken into account.

From Eqs. (21) and (22) one can easily verify that

\[
aa^\dagger = b\sqrt{\frac{B^*}{B}}\sqrt{\frac{B^*}{B}}\,b = [B + 1]. \quad (22)
\]

Furthermore using Eqs. (14) and (20) one can verify that

\[
[B, a^\dagger] = a^\dagger, \quad [B, a] = -a, \quad (25)
\]

which coincide with Eq. (2). Therefore the operators of Eq. (20) can be considered as a representation of the \( q \)-deformed boson operators in the usual (non-deformed) space \( |n\rangle_c \) of Eq. (17). The operators of Eq. (20) are referred to as \( q \)-deforming boson functionals. From Eqs. (11) and (24) it is also clear that in this representation the operator \( N \) is represented by the operator \( B \).

One can now build up the \( q \)-deformed oscillator states \( |n\rangle_q \) in terms of \( q \)-deforming boson functionals. Starting from Eq. (9) and using Eq. (20) one has

\[
|n\rangle_q = \frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle_q = \frac{1}{\sqrt{n!}}\sqrt{\frac{B}{B}}\sqrt{\frac{B}{B}} \ldots \sqrt{\frac{B}{B}}b^\dagger |0\rangle_c. \quad (26)
\]

Making use of the first relation in Eq. (23), all \( b^\dagger \) operators can be “shifted” to the right, giving

\[
|n\rangle_q = \frac{1}{\sqrt{n!}}\sqrt{\frac{[B][B - 1][B - 2] \ldots [B - n + 1]}{B(B - 1)(B - 2) \ldots (B - n + 1)}}(b^\dagger)^n|0\rangle_c
\]

\[
= \frac{1}{\sqrt{n!}}\sqrt{\frac{[n][n - 1][n - 2] \ldots [1]}{n(n - 1)(n - 2) \ldots 1}}\sqrt{n!}|n\rangle_c = |n\rangle_c, \quad (27)
\]

where in the middle step Eq. (17) has been used. We have therefore found that in this representation the \( q \)-deformed oscillator states coincide with the standard oscillator states, a quite remarkable result which will play an important role in what follows.
4 The Quantum Algebra $\text{su}_q(2)$

The quantum algebra $\text{su}_q(2)$ \cite{ref1, ref2, ref3} is a $q$-deformation of the Lie algebra $\text{su}(2)$. It is generated by the operators $L_+, L_-, L_0$, obeying the commutation relations (see \cite{ref4} and references therein)

$$[L_0, L_\pm] = \pm L_\pm,$$  \hspace{1cm} (28)

$$[L_+, L_-] = [2L_0] = \frac{q^{2L_0} - q^{-2L_0}}{q - q^{-1}},$$  \hspace{1cm} (29)

where $q$-numbers and $q$-operators are defined as in Eq. (4).

If the deformation parameter $q$ is not a root of unity (see the discussion preceding Eq. (6)) the finite-dimensional irreducible representation $D_{\ell}^{(q)}$ of $\text{su}_q(2)$ is determined by the highest weight vector $|\ell, \ell\rangle_q$ with

$$L_+|\ell, \ell\rangle_q = 0,$$  \hspace{1cm} (30)

and the basis states $|\ell, m\rangle_q$ are expressed as

$$|\ell, m\rangle_q = \sqrt{[\ell + m]!/[2\ell]![\ell - m]!} (L_-)^{\ell-m} |\ell, \ell\rangle_q.$$  \hspace{1cm} (31)

Then the explicit form of the irreducible representation (irrep) $D_{\ell}^{(q)}$ of the $\text{su}_q(2)$ algebra is determined by the equations

$$L_\pm|\ell, m\rangle_q = \sqrt{[\ell + m][\ell \pm m + 1]} |\ell, m \pm 1\rangle_q,$$  \hspace{1cm} (32)

$$L_0|\ell, m\rangle_q = m |\ell, m\rangle_q,$$  \hspace{1cm} (33)

and the dimension of the corresponding representation is the same as in the non-deformed case, i.e. $\text{dim}D_{\ell}^{(q)} = 2\ell + 1$ for $\ell = 0, \frac{1}{2}, 1, \frac{3}{2}, 2 \ldots$

The second-order Casimir operator of $\text{su}_q(2)$ is

$$C_2^{(q)} = \frac{1}{2} (L_+L_- + L_-L_+ + [2][L_0]^2)$$

$$= L_-L_+ + [L_0][L_0 + 1] = L_+L_- + [L_0][L_0 - 1],$$  \hspace{1cm} (34)

while its eigenvalues in the space of the irreducible representation $D_{\ell}^{(q)}$ are $[\ell][\ell + 1]$

$$C_2^{(q)}|\ell, m\rangle_q = [\ell][\ell + 1]|\ell, m\rangle_q.$$  \hspace{1cm} (35)

It has been suggested that rotational spectra of diatomic molecules \cite{ref5} and deformed nuclei (see \cite{ref6} and references therein) can be described by a phenomenological Hamiltonian based on the symmetry of the quantum algebra $\text{su}_q(2)$

$$H = \frac{\hbar^2}{2J_0} C_2^{(q)} + E_0,$$  \hspace{1cm} (36)

where $C_2^{(q)}$ is the second order Casimir operator of Eq. (34), $J_0$ is the moment of inertia for the non-deformed case $q \rightarrow 1$, and $E_0$ is the bandhead energy for a given band.
The eigenvalues of the Hamiltonian of Eq. (36) in the basis of Eq. (31) are then
\[ E_{\ell}^{(\tau)} = A[\ell][\ell + 1] + E_0, \] (37)
where the definition
\[ A = \frac{\hbar^2}{2J_0} \] (38)
has been used for brevity.

In the case with \( q = e^{\tau}, \tau \in \mathbb{R} \) the spectrum of the model Hamiltonian of Eq. (36) takes the form
\[ E_{\ell}^{(\tau)} = A \frac{\sinh(\ell\tau) \sinh((\ell + 1)\tau)}{\sinh^2(\tau)} + E_0, \quad q = e^{\tau}, \] (39)
while in the case with \( q = e^{i\tau}, \tau \in \mathbb{R} \) and \( q^n \neq 1, n \in \mathbb{N} \) the spectrum of the model Hamiltonian of Eq. (36) takes the form
\[ E_{\ell}^{(\tau)} = A \frac{\sin(\ell\tau) \sin((\ell + 1)\tau)}{\sin^2(\tau)} + E_0, \quad q = e^{i\tau}. \] (40)

It is known (see [4, 8, 9] and references therein) that only the spectrum of Eq. (40) exhibits behavior that is in agreement with experimentally observed rotational bands.

5 Representation of su\(_q\)(2) in Terms of q-Deformed Boson Operators

It has been found [5, 6] that the su\(_q\)(2) algebra of the last section can be represented in terms of two q-deformed boson operators like the ones introduced in Sec. 2. Indeed, one can consider as “building blocks” the independent q-deformed operators \( a_i^\dagger \) and \( a_i \), with \( i = 1, 2 \), which satisfy the commutation relations
\[ a_i a_i^\dagger - q^{\pm 1} a_i^\dagger a_i = q^{\mp N_i}, \] (41)
where \( N_i, i = 1, 2 \) are the corresponding q-deformed number operators, satisfying the commutation relations
\[ [N_i, a_i^\dagger] = a_i^\dagger, \quad [N_i, a_i] = -a_i. \] (42)

One can then verify that the operators
\[ L_+ = a_1^\dagger a_2, \quad L_- = a_1 a_2^\dagger, \quad L_0 = \frac{1}{2}(N_1 - N_2), \] (43)
do satisfy the commutation relations of Eqs. (28) and (29). In other words, Eq. (43) expresses a representation of the generators of su\(_q\)(2) in terms of q-deformed bosons.

In this representation the basis states are expressed as
\[ |n_1\rangle_q |n_2\rangle_q = \frac{(a_1^\dagger)^{n_1} (a_2^\dagger)^{n_2}}{\sqrt{n_1!} \sqrt{n_2!}} |0\rangle_q, \] (44)
With the identification

\[ n_1 = \ell + m, \quad n_2 = \ell - m, \]

the basis states are put into the form

\[ |\ell, m\rangle_q = \left( a_1^\dagger \right)^{\ell+m} \sqrt{\ell+m)!} \left( a_2^\dagger \right)^{\ell-m} \sqrt{\ell-m)!} |0\rangle_q, \]  

while the highest weight vector is

\[ |\ell, \ell\rangle_q = \left( a_1^\dagger \right)^{2\ell} \sqrt{2\ell)!} |0\rangle_q. \]

One can verify that the action of the operators of Eq. (43) on the states of Eq. (46) is described by Eqs. (32) and (33).

### 6 Connection of \( su_q(2) \) to the Lie Algebra \( su(2) \)

In this section we are going to use both the usual quantum mechanical operators of angular momentum, related to the Lie algebra \( su(2) \) and denoted by \( l_+, l_-, l_0 \), and the \( q \)-deformed ones, which are related to \( su_q(2) \) and denoted by \( L_+, L_-, L_0 \), as in Sections 4 and 5. For brevity we are going to call the operators \( l_+, l_-, l_0 \) “classical”, while the operators \( L_+, L_-, L_0 \) will be called “quantum”. For the “classical” basis the symbol \( |l, m\rangle_c \) will be used, while the “quantum” basis will be denoted by \( |\ell, m\rangle_q \), as in Sections 4 and 5. Therefore \( l \) and \( m \) are the quantum numbers related to the usual quantum mechanical angular momentum, which is characterized by the \( su(2) \) symmetry, while \( \ell \) and \( m \) are the quantum numbers related to the deformed angular momentum, which is characterized by the \( su_q(2) \) symmetry.

The “classical” operators satisfy the usual \( su(2) \) commutation relations

\[ [l_0, l_\pm] = \pm l_\pm, \quad [l_+, l_-] = 2l_0, \]

while the finite-dimensional irreducible representation \( D^l \) of \( su(2) \) is determined by the highest weight vector \( |l, l\rangle_c \) with

\[ l_+ |l, l\rangle_c = 0, \]  

and the basis states \( |l, m\rangle_c \) are expressed as

\[ |l, m\rangle_c = \sqrt{\frac{(l + m)!}{(2l)!(l - m)!}} (l_-)^{l-m} |l, l\rangle_c. \]

The action of the generators of \( su(2) \) on the vectors of the “classical” basis is described by

\[ l_\pm |l, m\rangle_c = \sqrt{(l \mp m)(l \pm m + 1)} |l, m \pm 1\rangle_c, \]

\[ l_0 |l, m\rangle_c = m |l, m\rangle_c, \]

the dimension of the corresponding representation being \( \dim D^l = 2l + 1 \) for \( l = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots \)
The second order Casimir operator of su(2) is
\[ C_2 = \frac{1}{2}(l_+l_- + l_-l_+) + l_0^2 = l_-l_+ + l_0(l_0 + 1) = l_+l_- + l_0(l_0 - 1), \] (53)
where the symbol 1 is used for the unit operator, while its eigenvalues in the space of the irreducible representation \( D^l \) are \( l(l + 1) \)
\[ C_2|l, m\rangle_c = l(l + 1)|l, m\rangle_c. \] (54)

One can build a representation of su(2) in terms of independent boson operators, for which the symbols \( b_i^\dagger \) and \( b_i \), with \( i = 1, 2 \) will be used, in a way similar to the one used in Sec. 3 for the harmonic oscillator. Indeed in the limit \( q \to 1 \) Eq. (41) is reduced into the usual commutation relation for independent boson operators
\[ [b_i, b_i^\dagger] = 1, \quad i = 1, 2, \] (55)
while Eq. (42) takes the form
\[ [B_i, b_i^\dagger] = b_i^\dagger, \quad [B_i, b_i] = -b_i, \quad i = 1, 2, \] (56)
where by \( B_i \) we denote the number operators, for which the following relations are valid
\[ b_i^\dagger b_i = B_i, \quad b_i b_i^\dagger = B_i + 1, \quad i = 1, 2. \] (57)
Furthermore in the limit \( q \to 1 \) Eq. (43) is reduced into
\[ l_+ = b_1^\dagger b_2, \quad l_- = b_1 b_2^\dagger, \quad l_0 = \frac{1}{2}(B_1 - B_2), \] (58)
which is the well known Schwinger realization of su(2). In other words, a representation of the generators of su(2) in terms of boson operators is obtained. One can verify that the operators given in Eq. (58) do satisfy the commutation relations of Eq. (48).

In this representation the basis states are expressed as
\[ |n_1\rangle_c|n_2\rangle_c = \frac{(b_1^\dagger)^{n_1}(b_2^\dagger)^{n_2}}{\sqrt{n_1!} \sqrt{n_2!}}|0\rangle_c, \] (59)
which can be viewed as the \( q \to 1 \) limit of Eq. (44). With the identification
\[ n_1 = l + m, \quad n_2 = l - m, \] (60)
the basis states are put into the form
\[ |l, m\rangle_c = \frac{(b_1^\dagger)^{l+m}(b_2^\dagger)^{l-m}}{\sqrt{(l + m)!} \sqrt{(l - m)!}}|0\rangle_c, \] (61)
which can be seen as the \( q \to 1 \) limit of Eq. (46).

One can easily verify that the operators of Eq. (58) act on the states of Eq. (61) in the way described by Eqs. (51) and (52).
One can now consider the connection between the “quantum” basis of Eq. (44) and the “classical” basis of Eq. (59). Using Eq. (27) one has

$$|n_1\rangle_q|n_2\rangle_q = \frac{(a_1^\dagger)^{n_1}}{\sqrt{n_1!}} \frac{(a_2^\dagger)^{n_2}}{\sqrt{n_2!}} |0\rangle_q = \frac{(b_1^\dagger)^{n_1}}{\sqrt{n_1!}} \frac{(b_2^\dagger)^{n_2}}{\sqrt{n_2!}} |0\rangle_c = |n_1\rangle_c|n_2\rangle_c,$$

(62)

or, in more compact form,

$$|n_1\rangle_q|n_2\rangle_q = |n_1\rangle_c|n_2\rangle_c.$$

(63)

In other words, in this boson representation the “quantum” states of su_q(2) coincide with the “classical” states of su(2). A direct consequence of this result is obtained by solving Eqs. (45) for \(\ell\) and m

$$\ell = \frac{n_1 + n_2}{2}, \quad m = \frac{n_1 - n_2}{2},$$

(64)

and Eqs. (60) for \(l\) and m

$$l = \frac{n_1 + n_2}{2}, \quad m = \frac{n_1 - n_2}{2}.$$

(65)

The fact that the “quantum” states and the “classical” states coincide, as seen in Eq. (63), means that from Eqs. (64) and (65) one obtains

$$\ell = l = \frac{n_1 + n_2}{2}, \quad m = m = \frac{n_1 - n_2}{2}.$$

(66)

In other words, the quantum numbers \(\ell\) and \(m\), appearing in the “quantum” states, are identical with the quantum numbers of the physical angular momentum, \(l\) and \(m\), appearing in the “classical” states. It should be remembered that these conclusions are valid in the case of \(q\) being not a root of unity, as already mentioned in Secs. 2 and 4.

In view of these remarks and using the identifications of Eqs. (45) and (60) one can put Eq. (63) into the form

$$|\ell, m\rangle_q = \frac{(a_1^\dagger)^{\ell + m}}{\sqrt{[\ell + m]!}} \frac{(a_2^\dagger)^{\ell - m}}{\sqrt{[\ell - m]!}} |0\rangle_q = \frac{(b_1^\dagger)^{\ell + m}}{\sqrt{(l + m)!}} \frac{(b_2^\dagger)^{\ell - m}}{\sqrt{(l - m)!}} = |l, m\rangle_c,$$

(67)

or, in more compact form,

$$|\ell, m\rangle_q = |l, m\rangle_c.$$

(68)

The action of the generators and of the second-order Casimir operator of su_q(2) on the “classical” states can be seen using Eqs. (32), (33), (35), (66), and (68)

$$L_\pm |l, m\rangle_c = L_\pm |\ell, m\rangle_q = \sqrt{[\ell \mp m][\ell \pm m + 1]} |\ell, m \pm 1\rangle_q = \sqrt{[l \mp m][l \pm m + 1]} |l, m \pm 1\rangle_c,$$

(69)

or, in short,

$$L_\pm |l, m\rangle_c = \sqrt{[l \mp m][l \pm m + 1]} |l, m \pm 1\rangle_c,$$

(70)

and in a completely analogous way

$$L_0 |l, m\rangle_c = m |l, m\rangle_c,$$

(71)

$$C_2^{(q)} |l, m\rangle_c = [l][l + 1] |l, m\rangle_c.$$

(72)
In a similar way one can obtain from Eqs. (51), (52), (54), (66), and (68) the action of the generators and of the second-order Casimir operator of su(2) on the “quantum” states

\[ l_\pm |\ell, m\rangle_q = \sqrt{(\ell \mp m)(\ell \pm m + 1)}|\ell, m \pm 1\rangle_q, \tag{73} \]

\[ l_0 |\ell, m\rangle_q = m|\ell, m\rangle_q, \tag{74} \]

\[ C_2 |\ell, m\rangle_q = \ell(\ell + 1)|\ell, m\rangle_q. \tag{75} \]

As a by-product, one can now show that the operators \( \hat{L}_+ \) and \( \hat{L}_- \) do not commute

\[ [\hat{L}_+, \hat{L}_-]|l, m\rangle_c = \hat{L}_+ \hat{L}_-|l, m\rangle_c - \hat{L}_- \hat{L}_+|l, m\rangle_c = \sqrt{(l - m)(l + m + 1)}|l, m + 1\rangle_c - (\sqrt{(l - m - 1)(l + m + 2)}\sqrt{(l - m)(l + m + 1)}|l, m + 2\rangle_c) \neq 0. \tag{76} \]

In the same way one can see that

\[ [\hat{L}_-, \hat{L}_-]|l, m\rangle_c \neq 0. \tag{77} \]

It should be mentioned at this point that the direct connection between the generators of su_\( q \)(2) and the generators of su(2) has been given in terms of \( q \)-deforming functionals in Refs. [20, 21], without any use of boson representations.

### 7 Rotational Invariance of the su_\( q \)(2) Hamiltonian

Using Eqs. (70), (72) one can verify that the operator \( C_2^{(q)} \) commutes with the generators \( L_+, L_- \), \( L_0 \) of su_\( q \)(2), i.e. that \( C_2^{(q)} \) is the second order Casimir operator of su_\( q \)(2). Indeed one has

\[ [C_2^{(q)}, L_+]|l, m\rangle_c = C_2^{(q)} L_+|l, m\rangle_c - L_+ C_2^{(q)}|l, m\rangle_c = C_2^{(q)} \sqrt{l + 1} l|l + 1\rangle_c + \sqrt{l - m} (l + m + 1)|l, m + 1\rangle_c - \sqrt{l - m} l|l + 1\rangle_c - \sqrt{l - m} (l + m + 1)|l, m + 1\rangle_c = 0. \tag{78} \]

In exactly the same way one can prove that

\[ [C_2^{(q)}, L_-]|l, m\rangle_c = 0, \tag{79} \]

while in addition, using Eqs. (71) and (72), one has

\[ [C_2^{(q)}, L_0]|l, m\rangle_c = C_2^{(q)} L_0|l, m\rangle_c - L_0 C_2^{(q)}|l, m\rangle_c = [l]|l + 1\rangle_c - m|l\rangle_c - m[l]|l + 1\rangle_c = 0. \tag{80} \]
Thus we have verified that the operator \( C(q)^2 \) is the second order Casimir operator of su\(_q\)(2). We are now going to prove that the operator \( C(q)^2 \) commutes also with the generators \( l_+ \), \( l_- \), \( l_0 \) of the usual su(2) algebra. Indeed using Eqs. (51) and (72) one has
\[
[C(q)^2, l_+] |l, m\rangle_c = C(q)^2 l_+ |l, m\rangle_c - l_+ C(q)^2 |l, m\rangle_c
\]
\[
= C(q)^2 \sqrt{(l - m)(l + m + 1)} |l, m\rangle_c - \sqrt{(l - m)(l + m + 1)} [l][l + 1] |l, m\rangle_c = 0. \tag{81}
\]
In exactly the same way one can prove that
\[
[C(q)^2, l_-] |l, m\rangle_c = 0, \tag{82}
\]
and the relation
\[
[C(q)^2, l_0] |l, m\rangle_c = 0 \tag{83}
\]
occurs from Eqs. (52) and (72).

The following comments are now in place:

a) The fact that the operator \( C(q)^2 \) commutes with the generators of su(2) implies that this operator is a function of the second order Casimir operator of su(2), given in Eq. (53). As a consequence, it should be possible to express the eigenvalues of \( C(q)^2 \), which are \([l][l+1]\) (as we have seen in Eq. (52) ), in terms of the eigenvalues of \( C_2 \), which are \( l(l + 1) \) (as we have seen in Eq. (54) ). This task will be undertaken in the next section.

b) Eqs. (81)-(83) also tell us that the Hamiltonian of Eq. (36) commutes with the generators of the usual su(2) algebra, i.e. it is rotationally invariant. The Hamiltonian of Eq. (36) does not break rotational symmetry. It corresponds to a function of the second order Casimir operator of the usual su(2) algebra. This function, however, has been chosen in an appropriate way, in order to guarantee that the Hamiltonian of Eq. (36) is also invariant under a more complicated symmetry, namely the symmetry su\(_q\)(2).

8 Exact Expansion of the su\(_q\)(2) Spectrum

Let us consider the spectrum of Eq. (40), which has been found relevant to rotational molecular and nuclear spectra, assuming for simplicity \( E_0 = 0 \) and \( \tau > 0 \). Since the Hamiltonian of Eq. (36) is invariant under su(2), as we have seen in the previous section, it should be possible in principle to express it as a function of the Casimir operator \( C_2 \) of the usual su(2) algebra. As a consequence, it should also be possible to express the eigenvalues of this Hamiltonian, given in Eq. (40), as a function of the eigenvalues of the Casimir operator of the usual su(2) algebra. This function, however, has been chosen in an appropriate way, in order to guarantee that the Hamiltonian of Eq. (36) is also invariant under a more complicated symmetry, namely the symmetry su\(_q\)(2).

The last expression is an even function of \((2l + 1)\). Therefore it is possible to express it as a power series in \((2l + 1)^2 = 4l(l + 1) + 1\). It turns out that the coefficients of the relevant
expansion in powers of $\ell(\ell + 1)$ can be expressed in terms of the spherical Bessel functions of the first kind $j_n(x)$ \[22\], which are determined through the generating function

$$\frac{1}{x} \cos \sqrt{x^2 - 2xt} = \sum_{n=0}^{\infty} j_n(x) \frac{t^n}{n!}, \quad (85)$$

and are characterized by the asymptotic behavior

$$j_n(x) \approx \frac{x^n}{(2n + 1)!!}, \quad x \ll 1. \quad (86)$$

Performing the substitutions

$$x = \tau, \quad t = -2\tau\ell(\ell + 1), \quad (87)$$

which imply

$$x^2 - 2xt = \tau^2(2\ell + 1)^2, \quad (88)$$

one gets the expression

$$\frac{1}{\tau} \cos((2\ell + 1)\tau) = \sum_{n=0}^{\infty} \frac{(-2\tau)^n}{n!} j_{n-1}(\tau) \{\ell(\ell + 1)\}^n, \quad (89)$$

which in the special case of $\ell = 0$ reads

$$\frac{1}{\tau} \cos \tau = j_{-1}(\tau), \quad (90)$$

in agreement with the definition \[22\]

$$j_{-1}(x) = \frac{\cos x}{x}. \quad (91)$$

Substituting Eqs. \[89\] and \[90\] in Eq. \[84\], and taking into account that \[22\]

$$j_0(x) = \frac{\sin x}{x}, \quad (92)$$

Eq. \[40\] takes the form

$$E^{(\tau)}_{\ell} = \frac{A}{j_0^2(\tau)} \sum_{n=0}^{\infty} \frac{(-1)^n(2\tau)^n}{(n + 1)!} j_n(\tau) \{\ell(\ell + 1)\}^{n+1}, \quad (93)$$

which is indeed an expansion in terms of $\ell(\ell + 1)$. 

13
9  Approximate Expansion of the $su_q(2)$ Spectrum

We are now going to consider an approximate form of this expansion, which will allow us to connect the present approach to the description of rotational spectra proposed by Amal’sky [11].

For “small deformation”, i.e. for $\tau \ll 1$, one can use the asymptotic expression of Eq. (86). Keeping only the terms of the lowest order one then obtains the following approximate series

$$E_\ell^{(\tau)} \approx A \sum_{n=0}^{\infty} \frac{(-1)^n(2\tau)^{2n}}{(n+1)(2n+1)!} \{\ell(\ell+1)\}^{n+1},$$

(94)

where use of the identity

$$2^n(n+1)!(2n+1)! = (n+1)(2n+1)!$$

(95)

has been made. The first few terms of this expansion are

$$E_\ell^{(\tau)} \approx A \left( \ell(\ell+1) - \frac{\tau^2}{3} \{\ell(\ell+1)\}^2 + \frac{2\tau^4}{45} \{\ell(\ell+1)\}^3 - \frac{\tau^6}{315} \{\ell(\ell+1)\}^4 + \ldots \right),$$

(96)

in agreement with the findings of Ref. [10].

One can now observe that the expansion appearing in Eq. (96) is similar to the power series of the function

$$\sin^2 x = \frac{1}{2} (1 - \cos 2x) = \sum_{k=1}^{\infty} (-1)^{k+1} 2^{2k-1} \frac{x^{2k}}{(2k)!},$$

(97)

Then, performing the auxiliary substitution

$$\xi = \sqrt{\ell(\ell+1)}, \quad \eta = \ell(\ell+1) = \xi^2,$$

(98)

one can put the expansion of Eq. (96) in the form

$$E_\ell^{(\tau)} \approx A \frac{\sin^2(\tau \xi)}{\tau^2} = \frac{\hbar^2}{2J_0} \frac{\sin^2(\tau \sqrt{\ell(\ell+1)})}{\tau^2}, \quad q = e^{i\tau}.$$  

(99)

This result is similar to the expression proposed for the unified description of nuclear rotational spectra by G. Amal’sky [11]

$$E_\ell = \varepsilon_0 \sin^2 \left( \frac{\pi}{N} \sqrt{\ell(\ell+1)} \right),$$

(100)

where $\varepsilon_0$ is a phenomenological constant ($\varepsilon_0 \approx 6.664$ MeV) which remains the same for all nuclei, while $N$ is a free parameter varying from one nucleus to the other.
10 Irreducible Tensor Operators under su\(_q\)(2)

A different path towards the construction of a Hamiltonian appropriate for the description of rotational spectra can be taken through the construction of irreducible tensor operators under su\(_q\)(2) \[12, 13\]. In this discussion we limit ourselves to real values of \(q\), i.e. to \(q = e^\tau\) with \(\tau\) being real, as in Refs. \[12, 13\].

An irreducible tensor operator of rank \(k\) is the set of \(2k + 1\) operators \(T^{(q)}_{k,\kappa}(k = k, k-1, k-2, \ldots, -k)\), which satisfy with the generators of the su\(_q\)(2) algebra the commutation relations \[12, 13\]

\[
[L_0, T^{(q)}_{k,\kappa}] = \kappa T^{(q)}_{k,\kappa},
\]

\[
[L_\pm, T^{(q)}_{k,\kappa}] q^\kappa = \sqrt{[k \mp \kappa][k \pm \kappa + 1]} T^{(q)}_{k,\kappa \pm 1} q^{-L_0},
\]

where \(q\)-commutators are defined by

\[
[A, B]_q = AB - q^\alpha BA.
\]

It is clear that in the limit \(q \to 1\) these commutation relations reduce to the usual ones, which occur in the definition of irreducible tensor operators under su(2). It should also be noticed that the operators

\[
R^{(q)}_{k,\kappa} = (-1)^\kappa q^{-\kappa}(T^{(q)}_{k,-\kappa})^\dagger,
\]

where \(^\dagger\) denotes Hermitian conjugation, satisfy the same commutation relations \[101\], \[102\] as the operators \(T^{(q)}_{k,\kappa}\), i.e. the operators \(R^{(q)}_{k,\kappa}\) also form an irreducible tensor operator of rank \(k\) under su\(_q\)(2).

We can construct an irreducible tensor operator of rank 1 using as building blocks the generators of su\(_q\)(2). This irreducible tensor operator will consist of the operators \(J_{+1}, J_{-1}, J_0\), which should satisfy the commutation relations

\[
[L_0, J_m] = m J_m,
\]

\[
[L_\pm, J_m] q^m = \sqrt{[1 \mp m][2 \pm m]} J_{m \pm 1} q^{-L_0},
\]

which are a special case of Eqs. \[101\], \[102\], while the relevant Hermitian conjugate operators will be

\[
(J_m)^\dagger = (-1)^m q^{-m} J_{-m},
\]

which is a consequence of Eq. \[103\]. It turns out \[12, 13, 23\] that the explicit form of the relevant operators is

\[
J_{+1} = -\frac{1}{\sqrt{2}} q^{-L_0} L_+,
\]

\[
J_{-1} = \frac{1}{\sqrt{2}} q^{-L_0} L_-,
\]

\[
J_0 = \frac{1}{2} (q L_+ L_- - q^{-1} L_- L_+) = \frac{1}{2} \left( q[2 L_0] + (q - q^{-1})(C_2^{(q)} - [L_0][L_0 + 1]) \right),
\]

while the Hermitian conjugate operators are

\[
(J_{+1})^\dagger = -q^{-1} J_{-1}, \quad (J_{-1})^\dagger = -q J_{+1}, \quad (J_0)^\dagger = J_0.
\]
It is clear that in the limit $q \to 1$ these results reduce to the usual expressions for spherical tensors of rank 1 under $\text{su}(2)$, formed out of the usual angular momentum operators

$$J_+ = \frac{-l_x + i l_y}{\sqrt{2}}, \quad J_- = \frac{l_x - i l_y}{\sqrt{2}}, \quad J_0 = l_0,$$  \hspace{1cm} (112)

$$(J_+)^\dagger = -J_-, \quad (J_-)^\dagger = -J_+, \quad (J_0)^\dagger = J_0.$$  \hspace{1cm} (113)

The commutation relations among the operators $J_{+1}, J_{-1}, J_0$ can be obtained using Eqs. (108)-(110) and (105), (106), as well as the fact that from Eq. (28) one has

$$[L_0, L_+] = L_+ \Rightarrow L_0 L_+ = L_+(L_0 + 1) \Rightarrow f(L_0)L_+ = L_+f(L_0 + 1),$$  \hspace{1cm} (114)

$$[L_0, L_-] = -L_- \Rightarrow L_0 L_- = L_-(L_0 - 1) \Rightarrow f(L_0)L_- = L_-f(L_0 - 1),$$  \hspace{1cm} (115)

where $f(x)$ is any function which can be written as a Taylor expansion in powers of $x$. Indeed one finds

$$[J_{+1}, J_0] = -q^{-2L_0+1}J_{+1}, \quad [J_{-1}, J_0] = q^{-2L_0-1}J_{-1}, \quad [J_{+1}, J_{-1}] = -q^{-2L_0}J_0.$$  \hspace{1cm} (116)

In the limit $q \to 1$ these results reduce to the usual commutation relations related to spherical tensor operators under $\text{su}(2)$

$$[J_+, J_0] = -J_+, \quad [J_-, J_0] = J_-, \quad [J_+, J_-] = -J_0.$$  \hspace{1cm} (117)

It is clear that the commutation relations of Eq. (116) are different from these of Eqs. (28), (29), as it is expected since the commutation relations of Eq. (117) are different from the usual commutation relations of $\text{su}(2)$, given in Eq. (18).

One can now try to build out of these operators the scalar square of the angular momentum operator. For this purpose one needs the definition of the tensor product of two irreducible tensor operators, which has the form $[12][23][24][25][26]$

$$[A_j(q) \otimes B_{j2}(q)]_{j,m}^{(1/q)} = \sum_{m_1, m_2} \langle j_1 m_1 j_2 m_2 | jm \rangle_{1/q} A_{j_1, m_1}^{(q)} B_{j_2, m_2}^{(q)}.$$  \hspace{1cm} (118)

One should observe that the irreducible tensor operators $A_j(q)$ and $B_{j2}(q)$, which correspond to the deformation parameter $q$, are combined into a new irreducible tensor operator $[A_j(q) \times B_{j2}(q)]_{j,m}$, which corresponds to the deformation parameter $1/q$, through the use of the deformed Clebsch–Gordan coefficients $\langle j_1 m_1 j_2 m_2 | jm \rangle_{1/q}$, which also correspond to the deformation parameter $1/q$.

Analytic expressions for several $q$-deformed Clebsch–Gordan coefficients, as well as their symmetry properties, can be found in Refs. [12][24]. Using the general formulae of Refs. [12][24] we derive here the Clebsch–Gordan coefficients which we will immediately need

$$\langle 1110 | 11 \rangle_q = q \sqrt{\frac{[2]}{[4]}}, \quad \langle 1011 | 11 \rangle_q = -q^{-1} \sqrt{\frac{[2]}{[4]}},$$  \hspace{1cm} (119)

$$\langle 101 - 1 | 1 - 1 \rangle_q = q \sqrt{\frac{[2]}{[4]}}, \quad \langle 1 - 110 | 1 - 1 \rangle_q = -q^{-1} \sqrt{\frac{[2]}{[4]}},$$  \hspace{1cm} (120)
\[ \langle 111 - 1|10 \rangle_q = \sqrt{\frac{2}{4}}, \quad (1 - 111|10 \rangle_q = -\sqrt{\frac{2}{4}}, \quad (1010|10 \rangle_q = (q - q^{-1})\sqrt{\frac{2}{4}}. \quad (121) \]

Using the definition of Eq. (118), the Clebsch–Gordan coefficients just given, as well as the commutation relations of Eq. (116), one finds the tensor products
\[
[J \otimes J]^{(1/q)}_{1,1} = \langle 1110|11 \rangle_{1/q} J_{1} + J_{0} J_{+1} \\
= -\sqrt{\frac{2}{4}} \left\{ q^{-2}L_{0} + (q - q^{-1})J_{0} \right\} J_{+1}, \quad (122)
\]
\[
[J \otimes J]^{(1/q)}_{1,-1} = \langle 101-1|1 \rangle_{1/q} J_{0} J_{-1} + (1 - 110|1 - 1)_{1/q} J_{-1} J_{0} \\
= -\sqrt{\frac{2}{4}} \left\{ q^{-2}L_{0} + (q - q^{-1})J_{0} \right\} J_{-1}, \quad (123)
\]
\[
[J \otimes J]^{(1/q)}_{1,0} = \langle 111 - 1|10 \rangle_{1/q} J_{1} J_{+1} + (1 - 1110|1 - 1)_{1/q} J_{+1} J_{1} + (1010|10 \rangle_{1/q} (J_{0})^2 \\
= -\sqrt{\frac{2}{4}} \left\{ q^{-2}L_{0} + (q - q^{-1})J_{0} \right\} J_{0}. \quad (124)
\]

We remark that all these tensor products are of the general form
\[
[J \otimes J]^{(1/q)}_{1, m} = -\sqrt{\frac{2}{4}} \left\{ q^{-2}L_{0} + (q - q^{-1})J_{0} \right\} J_{m} = -\sqrt{\frac{2}{4}} Z J_{m}, \quad m = 0, \pm 1 \quad (125)
\]

where by definition
\[
Z = q^{-2}L_{0} + (q - q^{-1})J_{0}. \quad (126)
\]

One can now prove that the operator \(Z\) is a scalar quantity, since it is a function of the second order Casimir operator of \(su_{q}(2)\), given in Eq. (134). Indeed one finds
\[
Z = q^{-2}L_{0} + (q - q^{-1})J_{0} = 1 + \frac{(q - q^{-1})^2}{2} C^{(q)}_{2}. \quad (127)
\]

Since \(Z\) is a scalar quantity, symmetric under the exchange \(q \leftrightarrow q^{-1}\) (as one can see from the last expression appearing in the last equation), Eq. (125) can be written in the form
\[
\left[ \frac{J}{Z} \otimes J \right]^{(1/q)}_{1,m} = -\sqrt{\frac{2}{4}} \left\{ J_{m} \right\} Z \Rightarrow [J' \otimes J']^{(1/q)}_{1,m} = -\sqrt{\frac{2}{4}} J'_{m}, \quad (128)
\]

where by definition
\[
J'_{m} = \frac{J_{m}}{Z}, \quad m = +1, 0, -1. \quad (129)
\]

It is clear that the operators \(J'_{m}\) also form an irreducible tensor operator, since \(Z\) is a function of the second order Casimir \(C^{(q)}_{2}\) of \(su_{q}(2)\), which commutes with the generators \(L_{+}, L_{-}, L_{0}\) of \(su_{q}(2)\), and therefore does not affect the commutation relations of Eqs. (105), (106), (107).
The scalar product of two irreducible tensor operators is defined as

\[
(A_j^{(q)} \cdot B_j^{(q)})^{(1/q)} = (-1)^{-j} \frac{1}{\sqrt{2j+1}} [A_j^{(q)} \times B_j^{(q)}]^{(1/q)}_{0,0} = \sum_m (-q)^{-m} A_j^{(q)} B_{j,-m}^{(q)}. \tag{130}
\]

Substituting the irreducible tensor operators \( J_m \) in this definition we obtain

\[
(J \cdot J)^{(1/q)} = -\frac{1}{3} [J \times J]^{(1/q)}_{0,0} = \frac{2}{[2]} C_2^{(q)} + \frac{(q - q^{-1})^2}{[2]^2} (C_2^{(q)})^2 = \frac{Z^2 - 1}{(q - q^{-1})^2}, \tag{131}
\]

where in the last step the identity

\[
Z^2 - 1 = (Z - 1)(Z + 1) = \frac{(q - q^{-1})^2}{[2]} C_2^{(q)} \left(2 + \frac{(q - q^{-1})^2}{[2]} C_2^{(q)}\right), \tag{132}
\]

has been used, obtained through use of Eq. (127). In the same way the irreducible tensor operators \( J'_m \) give the result

\[
(J' \cdot J')^{(1/q)} = \frac{1 - Z^{-2}}{(q - q^{-1})^2}. \tag{133}
\]

We have therefore determined the scalar square of the angular momentum operator. We can assume at this point that this quantity can be used (up to an overall constant) as the Hamiltonian for the description of rotational spectra, defining

\[
H = A \frac{1 - Z^{-2}}{(q - q^{-1})^2}, \tag{134}
\]

where \( A \) is a constant, which one can also write in the form

\[
A = \frac{\hbar^2}{2 J_0}, \tag{135}
\]

where \( J_0 \) is the moment of inertia.

The eigenvalues \( \langle Z \rangle \) of the operator \( Z \) in the basis \( |\ell, m \rangle \) can be easily found from the last expression given in Eq. (127), using the eigenvalues of the Casimir operator \( C_2^{(q)} \) in this basis, which are \([\ell][\ell + 1] \), as already mentioned in Sec. 4

\[
\langle Z \rangle = 1 + \frac{(q - q^{-1})^2}{[2]} [\ell][\ell + 1] = \frac{1}{2} (q^{2\ell+1} + q^{-2\ell-1}) = \frac{1}{2} ([2\ell + 2] - [2\ell]). \tag{136}
\]

The eigenvalues \( \langle (J \cdot J)^{(1/q)} \rangle \) of the scalar quantity \( (J \cdot J)^{(1/q)} \) can be found in a similar manner from Eq. (131)

\[
\langle (J \cdot J)^{(1/q)} \rangle = \frac{2}{[2]} [\ell][\ell + 1] + \frac{(q - q^{-1})^2}{[2]^2} [\ell]^2 [\ell + 1]^2 = \frac{[2\ell][2\ell + 2]}{[2]^2} = [\ell]_q [\ell + 1]_q^2, \tag{137}
\]

where by definition

\[
[x]_q^2 = \frac{q^{2x} - q^{-2x}}{q^2 - q^{-2}}. \tag{138}
\]
Finally, the eigenvalues $\langle H \rangle$ of the Hamiltonian can be found by substituting the eigenvalues of $Z$ from Eq. (136) into Eq. (134)

$$E = \langle H \rangle = A \frac{1}{(q - q^{-1})^2} \left( 1 - \frac{[2]^2}{(q^{2l+1} + q^{-2l-1})^2} \right)$$

$$= A \frac{1}{4 \sinh^2 \tau} \left( 1 - \frac{\cosh^2 \tau}{\cosh^2((2\ell + 1)\tau)} \right), \quad q = e^\tau,$$

where in the last step the identities

$$q - q^{-1} = 2 \sinh \tau, \quad [2] = q + q^{-1} = 2 \cosh \tau,$$

$$q^{2l+1} + q^{-2l-1} = 2 \cosh((2\ell + 1)\tau),$$

which are valid in the present case of $q = e^\tau$ with $\tau$ being real, have been used. In the same way one sees that

$$\langle Z \rangle = \frac{\cosh((2\ell + 1)\tau)}{\cosh \tau}.$$  \hspace{1cm} (142)

The following comments are now in place:

a) The last expression in Eq. (137) indicates that the eigenvalues of the scalar quantity $(J \cdot J)^{1/q}$ are equivalent to the eigenvalues of the Casimir operator of $\text{su}_q(2)$ (which are $l[l + 1]$), up to a change in the deformation parameter from $q$ to $q^2$.

b) From Eq. (136) it is clear that the eigenvalues of the scalar operator $Z$ go to the limiting value 1 as $q \to 1$. Therefore one can think of $Z$ as a “unity” operator. Furthermore the last expression in Eq. (136) indicates that $\langle Z \rangle$ is behaving like a “measure” of the unit of angular momentum in the deformed case.

11 Rotational Invariance of the $\text{su}_q(2)$ ITO Hamiltonian

In this section the method of Sec. 7 will be used once more. We wish to prove that the Hamiltonian of Eq. (134) commutes with the generators $l_+, l_-, l_0$ of the usual $\text{su}(2)$ algebra, i.e. with the usual angular momentum operators. Taking into account Eq. (127) we see that acting on the “classical” basis described in Sec. 6 we have

$$Z|l, m\rangle_c = \left( 1 + \frac{(q - q^{-1})^2}{[2]} C_2^{(q)} \right) |l, m\rangle_c = \left( 1 + \frac{(q - q^{-1})^2}{[2]} [l][l + 1] \right) |l, m\rangle_c.$$  \hspace{1cm} (143)

Then using Eq. (134) we see that

$$H|l, m\rangle_c = A \frac{1}{(q - q^{-1})^2} \left( 1 - \frac{1}{Z^2} \right) |l, m\rangle_c$$

$$= A \frac{1}{(q - q^{-1})^2} \left( 1 - \frac{1}{\left( 1 + \frac{(q - q^{-1})^2}{[2]} [l][l + 1] \right)^2} \right) |l, m\rangle_c.$$  \hspace{1cm} (144)
Using this result, as well as Eq. (51), one finds

\[
[H, l_+]|l, m\rangle_c = Hl_+|l, m\rangle_c - l_+H|l, m\rangle_c
\]

\[
= H\sqrt{(l - m)(l + m + 1)}|l, m\rangle_c
\]

\[-l_+ \frac{A}{(q - q^{-1})^2} \left( 1 - \frac{1}{\left( 1 + \frac{(q-q^{-1})^2}{2}[l][l+1] \right)^2} \right)|l, m\rangle_c
\]

\[-\sqrt{(l - m)(l + m + 1)} \frac{A}{(q - q^{-1})^2} \left( 1 - \frac{1}{\left( 1 + \frac{(q-q^{-1})^2}{2}[l][l+1] \right)^2} \right)|l, m+1\rangle_c = 0. \quad (145)
\]

In exactly the same way, using Eqs. (51), (52) and (144), one finds that

\[
[H, L_+]|l, m\rangle_c = 0, \quad [H, L_-]|l, m\rangle_c = 0, \quad [H, L_0]|l, m\rangle_c = 0.
\]

We have thus proved that the Hamiltonian of Eq. (134) is invariant under usual angular momentum. This result is expected, since the Hamiltonian is a function of the operator \(Z\), which in turn (as seen from Eq. (127) ) is a function of the second order Casimir operator of \(su_q(2)\), \(C^2(\varrho)\), which was proved to be rotationally invariant in Section 7.

Since the Hamiltonian of Eq. (134) is rotationally invariant, it should be possible to express it as a function of \(C^2\) (the second order Casimir operator of \(su(2)\) ). It should also be possible to express the eigenvalues of the Hamiltonian of Eq. (134) as a function of \(l(l+1)\), i.e. as a function of the eigenvalues of \(C^2\). This task will be undertaken in the following section.

For completeness we mention that using Eqs. (70), (71), and (144) one can prove in an analogous way that

\[
[H, J_+]|l, m\rangle_c = 0, \quad [H, J_-]|l, m\rangle_c = 0, \quad [H, J_0]|l, m\rangle_c = 0,
\]

i.e. that the Hamiltonian of Eq. (134) commutes with the generators of \(su_q(2)\) as well. Then from Eqs. (108)-(110) it is clear that in addition one has

\[
[H, J_+]|l, m\rangle_c = 0, \quad [H, J_-]|l, m\rangle_c = 0, \quad [H, J_0]|l, m\rangle_c = 0.
\]

Then from Eqs. (129) and (143) one furthermore obtains

\[
[H, J'_+]|l, m\rangle_c = 0, \quad [H, J'_-]|l, m\rangle_c = 0, \quad [H, J'_0]|l, m\rangle_c = 0.
\]

(149)
12 Exact Expansion of the su_q(2) ITO Spectrum

Since the Hamiltonian of Eq. (134) is invariant under su(2), as we have seen in the last section, it should be possible to write its eigenvalues (given in Eq. (139)) as an expansion in terms of ℓ(ℓ + 1). At this point it is useful to observe that in Eq. (139) an even function of the variable (2ℓ + 1) appears, which can therefore be expressed as a power series in (2ℓ + 1)^2 = 4ℓ(ℓ + 1) + 1. In this direction it turns out that one should use the Taylor expansion

$$\tanh x = \sum_{n=1}^{\infty} \frac{2^{2n}(2^{2n} - 1)B_{2n}}{(2n)!} x^{2n-1} = \sum_{n=0}^{\infty} \frac{2^{2n+2}(2^{2n+2} - 1)B_{2n+2}}{(2n+2)!} x^{2n+1}, \quad |x| < \frac{\pi}{2},$$

(150)

where B_n are the Bernoulli numbers \(^{22}\), defined through the generating function

$$\frac{x}{e^x - 1} = \sum_{n=0}^{\infty} B_n \frac{x^n}{n!},$$

(151)

the first few of them being

$$B_0 = 1, \quad B_1 = -\frac{1}{2}, \quad B_2 = \frac{1}{6}, \quad B_4 = -\frac{1}{30}, \quad B_6 = \frac{1}{42}, \quad B_8 = -\frac{1}{30}, \quad B_{10} = \frac{5}{66}, \ldots,$$

(152)

From Eq. (150) the following identities, concerning the derivatives of tanh x, occur

$$(\tanh x)' = \frac{1}{\cosh^2 x} = 1 - \tanh^2 x = \sum_{n=0}^{\infty} \frac{2^{2n+2}(2^{2n+2} - 1)B_{2n+2}}{(2n+2)!} x^{2n},$$

(153)

$$(\tanh x)'' = -\frac{2\tanh x}{\cosh^2 x} = -2\frac{\sinh x}{\cosh^2 x} = \sum_{n=0}^{\infty} \frac{2^{2n+4}(2^{2n+4} - 1)B_{2n+4}}{(2n+1)!(2n+4)} x^{2n+1}.$$  

(154)

From these equations the following auxiliary identities occur

$$\frac{\sinh x}{x \cosh^3 x} = -\frac{1}{2x}(\tanh x)'' = \sum_{n=0}^{\infty} \frac{2^{2n+3}(1 - 2^{2n+4})B_{2n+4}}{(2n+1)!(2n+4)} x^{2n},$$

(155)

$$\tanh^2 x = 1 - \frac{1}{\cosh^2 x} = \sum_{n=0}^{\infty} \frac{2^{2n+4}(1 - 2^{2n+4})B_{2n+4}}{(2n+2)!(2n+4)} x^{2n+2}.$$  

(156)

The expression for the energy, given in Eq. (139), can be put in the form

$$\frac{E}{A} = \left(\frac{\cosh^2 \tau}{\sinh^2 \tau}\right) \frac{1}{(2\tau)^2} \left\{ \frac{1}{\cosh^2 \tau} - \frac{1}{\cosh^2((2\ell + 1)\tau)} \right\}.$$  

(157)

Denoting

$$z = (2\ell + 1)\tau, \quad x = \ell(\ell + 1),$$

(158)

which imply

$$z^2 = (4x + 1)\tau^2, \quad z^{2n} = \tau^{2n} \sum_{k=0}^{n} \binom{n}{k} 2^{2k} x^k,$$  

(159)
Applying this general procedure in the case of Eq. (160), we obtain

\[
\frac{1}{\cosh^2((2\ell + 1)\tau)} = \frac{1}{\cosh^2 z} = \sum_{n=0}^{\infty} \frac{2^{2n+2}(2^{2n+2} - 1)B_{2n+2}}{(2n)!(2n + 2)} z^{2n}
\]

The double sum appearing in the last expression can be rearranged using the general procedure

\[
S = \sum_{n=0}^{\infty} a_n \sum_{k=0}^{n} b_{n,k} x^k
\]

\[
= a_0 b_{00} + a_1 (b_{10} + b_{11} x) + a_2 (b_{20} + b_{21} x + b_{22} x^2) + a_3 (b_{30} + b_{31} x + b_{32} x^2 + b_{33} x^3) + \ldots
\]

\[
= (a_0 b_{00} + a_1 b_{10} + a_2 b_{20} + a_3 b_{30} + \ldots) + (a_1 b_{11} + a_2 b_{21} + a_3 b_{31} + a_4 b_{41} + \ldots) x
\]

\[
+ (a_2 b_{22} + a_3 b_{32} + a_4 b_{42} + a_5 b_{52} + \ldots) x^2 + (a_3 b_{33} + a_4 b_{43} + a_5 b_{53} + a_6 b_{63} + \ldots) x^3 + \ldots
\]

\[
= \sum_{n=0}^{\infty} \sum_{k=n}^{\infty} a_k b_{k,n} x^k = \sum_{n=0}^{\infty} c_n x^n,
\]

where

\[
c_n = \sum_{k=n}^{\infty} a_k b_{k,n} = \sum_{k=0}^{\infty} a_{n+k} b_{n+k,n}.
\]

Applying this general procedure in the case of Eq. (160) we obtain

\[
\frac{1}{\cosh^2((2\ell + 1)\tau)} = \frac{1}{\cosh^2 z} = \sum_{n=0}^{\infty} c_n x^n,
\]

where

\[
c_n = \sum_{k=0}^{\infty} a_{n+k} b_{n+k,n} = \sum_{k=0}^{\infty} \frac{2^{2n+2k+2}(2^{2n+2k+2} - 1)B_{2n+2k+2}}{(2n + 2k)!(2n + 2k + 2)} \tau^{2n+2k} \binom{n+k}{n} 2^{2n}
\]

\[
= (2\tau)^{2n} \sum_{k=0}^{\infty} \frac{2^{2n+2k+2}(2^{2n+2k+2} - 1)B_{2n+2k+2}}{(2n + 2k)!(2n + 2k + 2)} \binom{n+k}{n} \tau^{2k}.
\]

The first term in Eq. (163) is

\[
c_0 = \sum_{k=0}^{\infty} \frac{2^{2k+2}(2^{2k+2} - 1)B_{2k+2}}{(2k)!(2k + 2)} \tau^{2k} = \frac{1}{\cosh^2 \tau}.
\]

Then one has

\[
\frac{1}{(2\tau)^2} \left\{ \frac{1}{\cosh^2 \tau} - \frac{1}{\cosh^2((2\ell + 1)\tau)} \right\} = -\frac{1}{(2\tau)^2} \sum_{n=1}^{\infty} c_n x^n
\]
\[-\frac{1}{(2\tau)^2} \sum_{n=0}^{\infty} c_{n+1} x^{n+1} = \sum_{n=0}^{\infty} d_n x^{n+1}, \quad (166)\]

where the coefficients \( d_n \) are

\[d_n = -\frac{1}{(2\tau)^2} c_{n+1} = \frac{(-1)^n (2\tau)^n}{(n+1)!} f_n(\tau), \quad n = 0, 1, 2, \ldots \quad (167)\]

with

\[f_n(\tau) = (-1)^{n+1} (2\tau)^n (n+1)! \sum_{k=0}^{\infty} \frac{2^{2n+2k+4}(2^{2n+2k+4} - 1) B_{2n+2k+4}}{(2n+2k+2)!(2n+2k+4)} \binom{n+k+1}{n+1} \tau^{2k}. \quad (168)\]

For \( n = 0 \) one has

\[f_0(\tau) = -\frac{2^{2k+4}(2^{2k+4} - 1) B_{2k+4}}{(2k+2)!(2k+4)} (k+1) \tau^{2k} = \frac{\sinh \tau}{\tau \cosh^3 \tau}, \quad (169)\]

where in the last step Eq. (155) has been used. It is worth noticing that

\[f_n(\tau) = (-1)^n (2\tau)^n \left( \frac{1}{\tau} \frac{d}{d \tau} \right)^n f_0(\tau). \quad (170)\]

With the help of Eqs. (166) and (167), the spectrum of Eq. (157) is put into the form

\[\frac{E}{A} = \left( \frac{\tau^2 \cosh^2 \tau}{\sinh^2 \tau} \right) \sum_{n=0}^{\infty} \frac{(-1)^n (2\tau)^n}{(n+1)!} f_n(\tau) (\ell(\ell + 1))^{n+1}, \quad (171)\]

since \( x = \ell(\ell + 1) \) from Eq. (158). It is clear that Eq. (171) is an expansion in terms of \( \ell(\ell + 1) \), as expected.

### 13 Approximate Expansion of the su\(_q(2)\) ITO Spectrum

In the limit of \( |\tau| << 1 \) one is entitled to keep in Eq. (168) only the term with \( k = 0 \). Then the function \( f_n(\tau) \) takes the form

\[f_n(\tau) \to \frac{(-1)^{n+1} 2^{2n+2}(2^{2n+4} - 1) B_{2n+4}}{(2n+1)!!(n+2)} \tau^n, \quad (172)\]

where the Bernoulli numbers appear again and use of the identity

\[(2n+2)! = 2^{n+1} (n+1)! (2n+1)!! \quad (173)\]

has been made. Taking into account the Taylor expansions

\[\sinh x = x + \frac{x^3}{3!} + \frac{x^5}{5!} + \cdots, \quad \cosh x = 1 + \frac{x^2}{2!} + \frac{x^4}{4!} + \cdots, \quad (174)\]
and keeping only the lowest order terms, one easily sees that Eq. (171) is put in the form

$$E \approx \frac{A}{\ell + 1} \sum_{n=0}^{\infty} \frac{2^{2n+4}(1 - 2^{2n+4})B_{2n+4}}{(2n + 2)!(2n + 4)}(2\tau)^{2n}\ell(\ell + 1)^{k+1},$$  \hspace{1cm} (175)

where use of the identity of Eq. (173) has been made once more and use of the fact that

$$\frac{\tau^2 \cosh^2 \tau}{\sinh^2 \tau} \approx 1 \quad \text{for} \quad |\tau| << 1$$  \hspace{1cm} (176)

has been made. Comparing this result with Eq. (156) and making the identifications

$$x = 2\tau \sqrt{\ell(\ell + 1)} = 2\tau \xi, \quad \xi = \sqrt{\ell(\ell + 1)},$$  \hspace{1cm} (177)

Eq. (175) is put into the compact form

$$E \approx \frac{A}{(2\tau)^2} \tanh^2(2\tau \sqrt{\ell(\ell + 1)}) = \frac{A}{(2\tau)^2} \tanh^2(2\tau \xi), \quad q = e^\tau.$$  \hspace{1cm} (178)

The extended form of the Taylor expansion of $E$ is easily obtained from Eq. (175)

$$E \approx A \left(\ell(\ell + 1) - \frac{2}{3}(2\tau)^2(\ell(\ell + 1))^2 + \frac{17}{45}(2\tau)^4(\ell(\ell + 1))^3 - \frac{62}{315}(2\tau)^6(\ell(\ell + 1))^4 + \cdots\right).$$  \hspace{1cm} (179)

Eq. (178) will be referred to as the “hyperbolic tangent formula”.

14 Numerical Tests

The formulae developed in the previous sections will be now tested against the experimental spectrum of the HF molecule, in which sizeable deviations from pure rotational behavior are observed. The data are taken from the R branch ($\ell \rightarrow \ell + 1$) and the P branch ($\ell \rightarrow \ell - 1$) of Ref. [27], using the equations [28]

$$E^R_\ell - E^P_\ell = E_{\ell+1}(v = 1) - E_{\ell-1}(v = 1),$$  \hspace{1cm} (180)

$$E^R_\ell - E^P_{\ell+2} = E_{\ell+2}(v = 0) - E_\ell(v = 0),$$  \hspace{1cm} (181)

where $v$ is the vibrational quantum number. The purpose of this study is two-fold:

a) To test the quality of the approximations used in Secs. 9 and 13.

b) To test the agreement between theoretical predictions and experimental data.

The standard rotational expansion,

$$E = A\ell(\ell + 1) + B(\ell(\ell + 1))^2 + C(\ell(\ell + 1))^3 + D(\ell(\ell + 1))^4 + \ldots,$$  \hspace{1cm} (182)

from which only the first two terms will be included in order to keep the number of parameters equal to two, as well as the Holmberg–Lipas two-parameter expression [14]

$$E = a(1 + b\ell(\ell + 1) - 1),$$  \hspace{1cm} (183)
which is known to give the best fits to experimental rotational nuclear spectra among all two-parameter expressions \[15\], will be included in the test for comparison. For brevity we are going to use the following terminology:
Model I for Eq. (40) (original $su_q(2)$ formula),
Model I’ for Eq. (99) (“the sinus formula”),
Model II for Eq. (139) (“the $su_q(2)$ irreducible tensor operator (ITO) formula”),
Model II’ for Eq. (178) (“the hyperbolic tangent formula”),
Model III for Eq. (182) (the standard rotational formula), and
Model IV for Eq. (183) (the Holmberg–Lipas formula).

It should be emphasized at this point that in models I and I’ the deformation parameter is a phase factor ($q = e^{i\tau}$, $\tau$ real), while in models II and II’ the deformation parameter is a real number ($q = e^\tau$, $\tau$ real). A consequence of this fact is the presence of trigonometric functions in models I and I’, while in models II and II’ hyperbolic functions appear.

The parameters resulting from the relevant least square fits, together with the quality measure

$$
\sigma = \sqrt{\frac{2}{\ell_{\text{max}}} \sum_{i=2}^{\ell_{\text{max}}} (E_{\text{exp}}(\ell) - E_{\text{th}}(\ell))^2}, \tag{184}
$$

where $\ell_{\text{max}}$ is the angular momentum of the highest level included in the fit, are listed in Table 1, while in Table 2 the theoretical predictions of all models for the $v = 0$ band of HF are listed together with the experimental spectrum.

From these tables the following observations can be made:

a) As seen in Tables 1 and 2, models I and I’ give results which are almost identical. The same is true for models II and II’. We therefore conclude that the approximations carried out in Secs. 5 and 10 are very accurate.

b) Models II and II’ appear to give the best results, followed by models I and I’. Model III gives reasonable results, while model IV gives the worst ones, a result which comes as a slight surprise, since model IV is known to provide the best fits of nuclear rotational spectra \[15\].

These observations lead to the following conclusions:

a) One can freely use model I’ in the place of model I, and model II’ in the place of model II, since the relevant approximations turn out to be very accurate. Models I’ and II’ have the advantage of providing simple analytic expressions for the energy.

b) The fact that models II and II’ are better than models I and I’ indicates that within the same symmetry ($su_q(2)$ in this case) it is possible to construct different rotational Hamiltonians characterized by different degrees of agreement with the data.

c) The relative failure of Model IV for molecular rotational spectra can be attributed to the fact that this model has been derived \[14\] from a Bohr–Mottelson Hamiltonian \[29\], which is certainly very appropriate for describing nuclear rotational spectra, but it is not necessarily equally appropriate for the description of molecular rotational spectra.

### 15 Discussion

The main results of the present work are the following:

a) The rotational invariance of the original $su_q(2)$ Hamiltonian \[8\], \[9\], \[10\] under the usual physical angular momentum has been proved explicitly and its connection to the formalism of Amal’sky \[11\] (“the sinus formula”) has been given.

b) An irreducible tensor operator (ITO) of rank one under $su_q(2)$ has been found and used, through $q$-deformed tensor product and $q$-deformed Clebsch–Gordan coefficient techniques \[12\], \[13\], \[23\], \[25\], for the construction of a new Hamiltonian appropriate for the description of rotational spectra, the $su_q(2)$ ITO Hamiltonian. The rotational invariance
of this new Hamiltonian under the usual physical angular momentum has been proved explicit-ily. Furthermore, an approximate simple closed expression (\textit{the hyperbolic tangent formula}) for the energy spectrum of this Hamiltonian has been found.

From the results of the present work it is clear that the $\text{su}_q(2)$ Hamiltonian, as well as the $\text{su}_q(2)$ ITO Hamiltonian, are complicated functions of the Casimir operator of the usual $\text{su}(2)$, i.e. of the square of the usual physical angular momentum. These complicated functions possess the $\text{su}_q(2)$ symmetry, in addition to the usual $\text{su}(2)$ symmetry. Matrix elements of these functions can be readily calculated in the deformed basis, but also in the usual physical basis. A similar study of a $q$-deformed quadrupole operator is called for.

**ACKNOWLEDGEMENTS**

The authors acknowledge support from the Bulgarian Ministry of Science and Education under Contracts No. Φ-415 and Φ-547.

**References**

[1] Chari, V.; Pressley, A. Quantum Groups; Cambridge University Press: Cambridge, 1994.

[2] Biedenharn, L. C.; Lohe, M. A. Quantum Group Symmetry and $q$-Tensor Algebras; World Scientific: Singapore, 1995.

[3] Klimyk, A.; and Schm"udgen, K. Quantum Groups and Their Representations; Springer: Berlin, 1997.

[4] Bonatsos, D.; Daskaloyannis, C. Prog Part Nucl Phys 1999, 43, 537-618.

[5] Biedenharn, L. C. J Phys A 1989, 22, L873-L878.

[6] Macfarlane, A. J. J Phys A 1989, 22, 4581-4588.

[7] Sun, C. P.; Fu, H. C. J Phys A 1989, 22, L983-L986.

[8] Bonatsos, D.; Raychev, P. P.; Roussev, R. P.; Smirnov, Yu. F. Chem Phys Lett 1990, 175, 300-306.

[9] Raychev, P. P.; Roussev, R. P.; Smirnov, Yu. F. J Phys G 1990, 16, L137-L141.

[10] Bonatsos, D.; Argyres, E. N.; Drenka, S. B.; Raychev, P. P.; Roussev, R. P.; Smirnov, Yu. F. Phys Lett B 1990, 251, 477-482.

[11] Amal’sky, G. M. Yad Fiz 1993, 56, 70-85 [Phys At Nucl 1993, 56, 1190-1200].

[12] Smirnov, Yu. F.; Tolstoy, V. N.; Kharitonov, Yu. I. Yad Fiz 1991, 53, 959-980 [Sov J Nucl Phys 1991, 53, 593-605].

[13] Smirnov, Yu. F.; Tolstoy, V. N.; Kharitonov, Yu. I. Yad Fiz 1993, 56, 223-244 [Phys At Nucl 1993, 56, 690-700].

[14] Holmberg, P.; Lipas, P. O. Nucl Phys A 1968, 117, 552-560.
[15] Casten, R. F. Nuclear Structure from a Simple Perspective; Oxford University Press: Oxford, 1990.

[16] Song, X. C. J Phys A 1990, 23, L821-L825.

[17] Kulish, P. P.; Reshetikhin, N. Yu. Zap Nauchn Semin LOMI 1981, 101, 101-110.

[18] Sklyanin, E. K. Funct Anal Appl 1982, 16, 263-270.

[19] Jimbo, M. Lett Math Phys 1986, 11, 247-252.

[20] Curtright, T. L.; Ghandour, G. I.; Zachos, C. K. J Math Phys 1991, 32, 676-688.

[21] Curtright, T. L.; Zachos, C. K. Phys Lett B 1990, 243, 237-244.

[22] Abramowitz, M.; Stegun, I. A. Handbook of Mathematical Functions; Dover: New York, 1965.

[23] Raychev, P. P.; Roussev, R. P.; Terziev, P. A.; Bonatsos, D.; Lo Iudice, N. J Phys A 1996, 29, 6939-6949.

[24] Smirnov, Yu. F.; Tolstoy, V. N.; Kharitonov, Yu. I. Yad Fiz 1991, 53, 1746-1771 [Sov J Nucl Phys 1991, 53, 1068-1086].

[25] Smirnov, Yu. F.; Tolstoy, V. N.; Kharitonov, Yu. I. Yad Fiz 1992, 55, 2863-2874 [Sov J Nucl Phys 1992, 55, 1599-1604].

[26] Raychev, P. P.; Roussev, R. P.; Lo Iudice, N.; Terziev, P. A. J Phys G 1998, 24, 1931-1943.

[27] Mann, D. E., Thrush, B. A.; Lide Jr., D. R.; Ball, J. J.; Acquista, N. J Chem Phys 1961, 34, 420-431.

[28] Barrow, G. M. Introduction to Molecular Spectroscopy; McGraw–Hill: London, 1962.

[29] Bohr, A.; Mottelson, B. R. Nuclear Structure; World Scientific: Singapore, 1998; Vol. II.
Table 1: Parameter values and quality measure $\sigma$ (Eq. (184)) for models I (Eq. (40)), I' (Eq. (99)), II (Eq. (139)), II' (Eq. (178)), III (Eq. (182)), and IV (Eq. (183)), obtained from least square fits (shown in Table 2) to the experimental spectrum of the $v = 0$ band of HF, taken from Ref. [27] through Eqs. (180), (181).

|       | I    | I'   | II   | II'  | III  | III  | IV   | IV   |
|-------|------|------|------|------|------|------|------|------|
| $A$ (cm$^{-1}$) | 20.553 | 20.554 | 20.559 | 20.559 | 20.550 | 20.550 | 93982 |
| $10^2 \tau$ | 1.742 | 1.742 | 0.623 | 0.623 | 0.204 | 0.204 | 0.438 |
| $\sigma$ (cm$^{-1}$) | 0.072 | 0.072 | 0.048 | 0.051 | 0.163 | 0.163 | 0.313 |

Table 2: Theoretical predictions of models I (Eq. (40)), I' (Eq. (99)), II (Eq. (139)), II' (Eq. (178)), III (Eq. (182)), and IV (Eq. (183)), obtained from least square fits to the experimental spectrum (exp.) of the $v = 0$ band of HF, taken from Ref. [27] through Eqs. (180), (181). All energies are given in cm$^{-1}$. The relevant model parameters and quality measure $\sigma$ (Eq. (184)) are given in Table 1.

| $\ell$ | exp. | I    | I'   | II   | II'  | III  | IV   |
|--------|------|------|------|------|------|------|------|
| 2      | 123.33 | 123.25 | 123.25 | 123.29 | 123.27 | 123.23 | 123.34 |
| 4      | 410.34 | 410.25 | 410.25 | 410.35 | 410.32 | 410.18 | 410.52 |
| 6      | 859.69 | 859.60 | 859.60 | 859.73 | 859.72 | 859.49 | 860.04 |
| 8      | 1469.2 | 1469.1 | 1469.1 | 1469.3 | 1469.3 | 1469.0 | 1469.6 |
| 10     | 2235.9 | 2235.9 | 2235.9 | 2236.0 | 2236.0 | 2235.8 | 2236.2 |
| 12     | 3156.1 | 3156.1 | 3156.1 | 3156.1 | 3156.1 | 3156.1 | 3156.1 |
| 14     | 4225.3 | 4225.4 | 4225.4 | 4225.3 | 4225.2 | 4225.5 | 4224.9 |
| 16     | 5438.4 | 5438.5 | 5438.5 | 5438.3 | 5438.3 | 5438.6 | 5438.0 |
| 18     | 6789.6 | 6789.5 | 6789.5 | 6789.6 | 6789.7 | 6789.4 | 6790.0 |