

Quantum Groups in Nuclear Spectra

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Abstract.

We demonstrate how quantum algebras (quantum groups), which are non-linear generalizations of the usual Lie algebras, can be used for constructing nuclear Hamiltonians which, in addition to the deformed symmetry $su_q(2)$, also obey the usual $su(2)$ symmetry underlying physical angular momentum. In particular, the rotational invariance under the usual physical angular momentum of the $su_q(2)$ Hamiltonian for the description of rotational nuclear spectra is explicitly proved and a connection of this Hamiltonian to the formalisms of Amal'sky and Harris is provided. Furthermore, 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, a simple closed expression for its energy spectrum (the “hyperbolic tangent formula”) is introduced, and its connection to the Harris formalism is established. Numerical tests in a series of Th isotopes are provided. The way in which the same techniques can be used for the description of magic numbers and supershells in metal clusters is also briefly mentioned.

1 Introduction

Quantum algebras [1–3] have started finding applications in the description of symmetries of physical systems over the last years [4]. 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 nuclear spectra [5] and its relation to the Variable Moment of Inertia Model [6] 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?

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.

After a brief introduction to the $su_q(2)$ formalism in Section 2, we prove explicitly in Section 3 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 generators of $su_q(2)$ are expressed in terms of the generators of $su(2)$. In addition, it turns out that the angular momentum quantum numbers appearing in the description of the irreducible representations (irreps) of $su_q(2)$ are exactly the same as the ones appearing in the irreps of $su(2)$, establishing an one-to-one correspondence between the two sets of irreps (in the generic case in which the deformation parameter q is not a root of unity).

Taking advantage of the results of Section 3, we write in Section 4 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 5, leads to a closed energy formula for rotational spectra introduced by Amal'sky [7]. The study of analytic expressions for the moment of inertia and the rotational frequency based on the closed formula of Section 5 leads in Section 6 to a connection between the present approach and the Harris formalism [8].

We then turn in Section 7 into the study of irreducible tensor operators under $su_q(2)$ [9, 10], 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 [9]. 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 $\text{su}_q(2)$ ITO Hamiltonian does commute with the generators of the usual $\text{su}(2)$ algebra is shown in Section 8. Based on the results of Section 8, we express in Section 9 the eigenvalues of the $\text{su}_q(2)$ 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 10, leads to a simple closed formula for the spectrum (the “hyperbolic tangent formula”), which is used in Section 11 in order to obtain analytic expressions for the moment of inertia and the rotational frequency, leading to a connection of the present results to the Harris formalism [8].

Finally in Section 12 all the exact and closed approximate energy formulae obtained above are compared to the experimental spectra of a series of Th isotopes, as well as to the results provided by the usual rotational expansion and by the Holmberg–Lipas formula [11], which is probably the best two-parameter formula for the description of rotational nuclear spectra [12]. A discussion of the present results and plans for future work are given in Section 13.

2 The Quantum Algebra $\text{su}_q(2)$

The quantum algebra $\text{su}_q(2)$ [13–15] 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 [4] and references therein)

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

where q -numbers and q -operators are defined by

$$[x] = \frac{q^x - q^{-x}}{q - q^{-1}}. \quad (2)$$

There are two distinct cases for the domain of the deformation parameter:

a) $q = e^{\tau}$, $\tau \in \mathbf{R}$, in which

$$[x] = \frac{\sinh \tau x}{\sinh \tau}, \quad (3)$$

b) $q = e^{i\tau}$, $\tau \in \mathbf{R}$, in which

$$[x] = \frac{\sin \tau x}{\sin \tau}. \quad (4)$$

In both cases one has

$$[x] \rightarrow x \quad \text{as} \quad q \rightarrow 1. \quad (5)$$

If the deformation parameter q is not a root of unity [q is a root of unity in case b) if one has $q^n = 1, n \in \mathbf{N}$] the finite-dimensional irreducible representation $D_{(q)}^\ell$ of $\text{su}_q(2)$ is determined by the highest weight vector $|\ell, \ell\rangle_q$ with

$$L_+|\ell, \ell\rangle_q = 0, \tag{6}$$

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

$$|\ell, m\rangle_q = \sqrt{\frac{[\ell + m]!}{[2\ell]![\ell - m]!}} (L_-)^{\ell - m} |\ell, \ell\rangle_q, \tag{7}$$

where $[n]! = [n][n - 1] \dots [1]$ is the notation for the q -factorial. Then the explicit form of the irreducible representation (irrep) $D_{(q)}^\ell$ of the $\text{su}_q(2)$ algebra is determined by the equations

$$L_\pm|\ell, m\rangle_q = \sqrt{[\ell \mp m][\ell \pm m + 1]} |\ell, m \pm 1\rangle_q, \quad L_0|\ell, m\rangle_q = m|\ell, m\rangle_q, \tag{8}$$

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

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

$$\begin{aligned} C_2^{(q)} &= \frac{1}{2}(L_+L_- + L_-L_+ + [2][L_0]^2) \\ &= L_-L_+ + [L_0][L_0 + 1] = L_+L_- + [L_0][L_0 - 1], \end{aligned} \tag{9}$$

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

$$C_2^{(q)}|\ell, m\rangle_q = [\ell][\ell + 1]|\ell, m\rangle_q. \tag{10}$$

It has been suggested (see [4,5] and references therein) that rotational spectra of deformed nuclei and diatomic molecules can be described by a phenomenological Hamiltonian based on the symmetry of the quantum algebra $\text{su}_q(2)$

$$H = \frac{\hbar^2}{2\mathcal{J}_0} C_2^{(q)} + E_0, \tag{11}$$

where $C_2^{(q)}$ is the second order Casimir operator of Eq. (9), \mathcal{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. (11) in the basis of Eq. (7) are then

$$E_\ell^{(\tau)} = A[\ell][\ell + 1] + E_0, \tag{12}$$

where the definition

$$A = \frac{\hbar^2}{2\mathcal{J}_0} \quad (13)$$

has been used for brevity.

In the case with $q = e^\tau$, $\tau \in \mathbf{R}$ the spectrum of the model Hamiltonian of Eq. (11) takes the form

$$E_\ell^{(\tau)} = A \frac{\sinh(\ell\tau) \sinh((\ell+1)\tau)}{\sinh^2(\tau)} + E_0, \quad q = e^\tau \quad (14)$$

while in the case with $q = e^{i\tau}$, $\tau \in \mathbf{R}$ and $q^n \neq 1$, $n \in \mathbf{N}$ the spectrum of the model Hamiltonian of Eq. (11) takes the form

$$E_\ell^{(\tau)} = A \frac{\sin(\ell\tau) \sin((\ell+1)\tau)}{\sin^2(\tau)} + E_0, \quad q = e^{i\tau}. \quad (15)$$

It is known (see [4, 5] and references therein) that only the spectrum of Eq. (15) exhibits behavior that is in agreement with experimentally observed rotational bands.

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

In this section we are going to use both the usual quantum mechanical operators of angular momentum, denoted by \hat{l}_+ , \hat{l}_- , \hat{l}_0 , and the q -deformed ones, which are related to $\text{su}_q(2)$ and denoted by \hat{L}_+ , \hat{L}_- , \hat{L}_0 , as in Section 2. In this section we are going to use hats ($\hat{}$) for the operators, in order to give emphasis to the distinction between the operators and their eigenvalues. For brevity we are going to call the operators \hat{l}_+ , \hat{l}_- , \hat{l}_0 “classical”, while the operators \hat{L}_+ , \hat{L}_- , \hat{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 Section 2. Therefore l and m are the quantum numbers related to the usual quantum mechanical angular momentum, which is characterized by the $\text{su}(2)$ symmetry, while ℓ and m are the quantum numbers related to the deformed angular momentum, which is characterized by the $\text{su}_q(2)$ symmetry.

The “classical” operators satisfy the usual $\text{su}(2)$ commutation relations

$$[\hat{l}_0, \hat{l}_\pm] = \pm \hat{l}_\pm, \quad [\hat{l}_+, \hat{l}_-] = 2\hat{l}_0, \quad (16)$$

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

$$\hat{l}_+ |l, l\rangle_c = 0, \quad (17)$$

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

$$|l, m\rangle_c = \sqrt{\frac{(l+m)!}{(2l)!(l-m)!}} (\hat{l}_-)^{l-m} |l, l\rangle_c. \quad (18)$$

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

$$\hat{l}_\pm |l, m\rangle_c = \sqrt{(l \mp m)(l \pm m + 1)} |l, m \pm 1\rangle_c, \quad \hat{l}_0 |l, m\rangle_c = m |l, m\rangle_c, \quad (19)$$

the dimension of the corresponding representation being $\dim D^l = 2l + 1$ for $l = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \dots$

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

$$\hat{C}_2 = \frac{1}{2}(\hat{l}_+ \hat{l}_- + \hat{l}_- \hat{l}_+) + \hat{l}_0^2 = \hat{l}_- \hat{l}_+ + \hat{l}_0(\hat{l}_0 + 1) = \hat{l}_+ \hat{l}_- + \hat{l}_0(\hat{l}_0 - 1), \quad (20)$$

where the symbol 1 is used for the unit operator, while its eigenvalues in the space of the irreducible representation D^l are $l(l+1)$

$$\hat{C}_2 |l, m\rangle_c = l(l+1) |l, m\rangle_c. \quad (21)$$

It is useful to introduce the operator \hat{l} through the definition

$$\hat{C}_2 \equiv \hat{l}(\hat{l} + 1). \quad (22)$$

Insisting that \hat{l} should be a positive operator one then has by solving the relevant quadratic equation and keeping only the positive sign in front of the square root [16]

$$\hat{l} = \frac{1}{2}(-1 + \sqrt{1 + 4\hat{C}_2}). \quad (23)$$

The action of the operator \hat{l} on the vectors of the “classical” basis is then given by

$$\begin{aligned} \hat{l} |l, m\rangle_c &= \frac{1}{2}(-1 + \sqrt{1 + 4\hat{C}_2}) |l, m\rangle_c \\ &= \frac{1}{2}(-1 + \sqrt{1 + 4l(l+1)}) |l, m\rangle_c \\ &= \frac{1}{2}(-1 + \sqrt{(2l+1)^2}) |l, m\rangle_c = \frac{1}{2}(-1 + 2l+1) |l, m\rangle_c = l |l, m\rangle_c, \end{aligned} \quad (24)$$

where again only the positive value of the square root has been taken into account.

In this “classical” environment one can introduce the operators [16, 17]

$$\hat{L}_+ = \sqrt{\frac{[\hat{l} + \hat{l}_0][\hat{l} - \hat{l}_0 + 1]}{(\hat{l} + \hat{l}_0)(\hat{l} - \hat{l}_0 + 1)}} \hat{l}_+, \quad \hat{L}_- = \hat{l}_- \sqrt{\frac{[\hat{l} + \hat{l}_0][\hat{l} - \hat{l}_0 + 1]}{(\hat{l} + \hat{l}_0)(\hat{l} - \hat{l}_0 + 1)}}, \quad (25)$$

$$\hat{L}_0 = \hat{l}_0,$$

where square brackets denote q -operators, as defined in Eq. (2).

One can easily verify that the action of these operators on the vectors of the “classical” basis is given by

$$\hat{L}_\pm |l, m\rangle_c = \sqrt{[l \mp m][l \pm m + 1]} |l, m \pm 1\rangle_c, \quad \hat{L}_0 |l, m\rangle_c = m |l, m\rangle_c. \quad (26)$$

One can also verify that that the operators \hat{L}_+ and \hat{l}_+ do not commute

$$[\hat{L}_+, \hat{l}_+] |l, m\rangle_c \neq 0. \quad (27)$$

This result is expected if one considers Eq. (25): The operator \hat{l}_+ does commute with itself and with the operator \hat{l} , which is a function of the relevant Casimir operator, as Eq. (23) indicates, but it does not commute with the operator \hat{l}_0 , as Eq. (16) shows. In the same way one can see that

$$[\hat{L}_-, \hat{l}_-] |l, m\rangle_c \neq 0. \quad (28)$$

One can now prove that the “new” operators satisfy the commutation relations of Eq. (1)

$$[\hat{L}_0, \hat{L}_+] |l, m\rangle_c = \hat{L}_+ |l, m\rangle_c, \quad [\hat{L}_0, \hat{L}_-] |l, m\rangle_c = -\hat{L}_- |l, m\rangle_c, \quad (29)$$

$$[\hat{L}_+, \hat{L}_-] |l, m\rangle_c = [2\hat{L}_0] |l, m\rangle_c.$$

One can also see that the operator

$$\hat{C} = \hat{L}_- \hat{L}_+ + [\hat{L}_0][\hat{L}_0 + 1] \quad (30)$$

acts on the vectors of the “classical” basis as

$$\hat{C} |l, m\rangle_c = [l][l + 1] |l, m\rangle_c. \quad (31)$$

Using Eqs. (26), (31) one can now prove that the operator \hat{C} commutes with the generators \hat{L}_+ , \hat{L}_- , \hat{L}_0 of $\text{su}_q(2)$, i.e. that \hat{C} is the second order Casimir operator of $\text{su}_q(2)$. Indeed one can verify that

$$[\hat{C}, \hat{L}_+] |l, m\rangle_c = 0, \quad [\hat{C}, \hat{L}_-] |l, m\rangle_c = 0, \quad [\hat{C}, \hat{L}_0] |l, m\rangle_c = 0. \quad (32)$$

Thus we have proved that the operator \hat{C} is the second order Casimir operator of $\text{su}_q(2)$. We are now going to prove that the operator \hat{C} commutes also with the

generators \hat{l}_+ , \hat{l}_- , \hat{l}_0 of the usual $\text{su}(2)$ algebra. Indeed using Eqs. (19) and (31) one can verify that

$$[\hat{C}, \hat{l}_+]|l, m\rangle_c = 0, \quad [\hat{C}, \hat{l}_-]|l, m\rangle_c = 0, \quad [\hat{C}, \hat{l}_0]|l, m\rangle_c = 0. \quad (33)$$

The following comments are now in place:

a) The fact that the operator \hat{C} , which will be from now on denoted by $\hat{C}_2^{(q)}$, commutes with the generators of $\text{su}(2)$ implies that this operator is a function of the second order Casimir operator of $\text{su}(2)$, given in Eq. (20). As a consequence, it should be possible to express the eigenvalues of $\hat{C}_2^{(q)}$, which are $[l][l+1]$ (as we have seen in Eq. (31)), in terms of the eigenvalues of \hat{C}_2 , which are $l(l+1)$ (as we have seen in Eq. (21)). This task will be undertaken in the next section.

b) Eq. (33) also tells us that the Hamiltonian of Eq. (11) commutes with the generators of the usual $\text{su}(2)$ algebra, i.e. it is rotationally invariant. The Hamiltonian of Eq. (11) does not break rotational symmetry. It corresponds to a function of the second order Casimir operator of the usual $\text{su}(2)$ algebra. This function, however, has been chosen in an appropriate way, in order to guarantee that the Hamiltonian of Eq. (11) is also invariant under a more complicated symmetry, namely the symmetry $\text{su}_q(2)$.

c) From the contents of the present section it is also clear that the irrep $D_{(q)}^\ell$ of $\text{su}_q(2)$ and the irrep D^l of $\text{su}(2)$ have the same structure, the relevant states being in an one to one correspondence to each other. The similarity between Eqs. (26) and (19) implies that the distinction between the ‘‘classical’’ basis of the present section and the ‘‘quantum’’ basis of Section 2 turns out to be unnecessary, as well as that the quantum numbers ℓ and m can be identified with the usual angular momentum quantum numbers l and m .

d) These conclusions are valid in the case of q being not a root of unity, as already mentioned in Section 2.

4 Exact Expansion of the $\text{su}_q(2)$ Spectrum

Let us consider the spectrum of Eq. (15), which has been found relevant to rotational nuclear and molecular spectra, assuming for simplicity $E_0 = 0$ and $\tau > 0$. Since the Hamiltonian of Eq. (11) is invariant under $\text{su}(2)$, 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 $\text{su}(2)$ algebra. As a consequence, it should also be possible to express the eigenvalues of this Hamiltonian, given in Eq. (15), as a function of the eigenvalues of the Casimir operator of the usual $\text{su}(2)$, i.e. as a function of $l(l+1)$. This is a nontrivial task, since in Eq. (15) two different functions of the variable ℓ appear, while we are in need of a single function of the variable $l(l+1)$, which is related to the length of the angular momentum vector.

It turns out that Eq. (15) takes the form

$$E_\ell^{(\tau)} = \frac{A}{j_0^2(\tau)} \sum_{n=0}^{\infty} \frac{(-1)^n (2\tau)^n}{(n+1)!} j_n(\tau) \{\ell(\ell+1)\}^{n+1}, \quad (34)$$

where $j_n(x)$ denote the spherical Bessel functions of the first kind [18]. Eq. (34) is indeed an expansion in terms of $\ell(\ell+1)$.

5 Approximate Expansion of the $\text{su}_q(2)$ 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 nuclear spectra proposed by Amal'sky [7].

For "small deformation", i.e. for $\tau \ll 1$, and taking advantage of the relevant asymptotic form of the spherical Bessel functions of the first kind $j_n(x)$ [18], one obtains the following approximate series

$$E_\ell^{(\tau)} \approx A \sum_{n=0}^{\infty} \frac{(-1)^n (2\tau)^{2n}}{(n+1)(2n+1)!} \{\ell(\ell+1)\}^{n+1}, \quad (35)$$

the first few terms of which are

$$E_\ell^{(\tau)} \approx A \left(\ell(\ell+1) - \frac{\tau^2}{3} \{\ell(\ell+1)\}^2 + \frac{2\tau^4}{45} \{\ell(\ell+1)\}^3 - \frac{\tau^6}{315} \{\ell(\ell+1)\}^4 + \dots \right), \quad (36)$$

in agreement with the findings of Ref. [6].

Introducing the notation

$$\xi = \sqrt{\ell(\ell+1)}, \quad \eta = \ell(\ell+1) = \xi^2, \quad (37)$$

one can put the expansion of Eq. (35) in the form

$$E_\ell^{(\tau)} \approx A \frac{\sin^2(\tau\xi)}{\tau^2} = \frac{\hbar^2}{2\mathcal{J}_0} \frac{\sin^2(\tau\sqrt{\ell(\ell+1)})}{\tau^2}. \quad (38)$$

This result is similar to the expression proposed for the unified description of nuclear rotational spectra by G. Amal'sky [7]

$$E_\ell = \varepsilon_0 \sin^2 \left(\frac{\pi}{N} \sqrt{\ell(\ell+1)} \right), \quad (39)$$

where ε_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.

6 Analytic Expressions Based on the Approximate Expansion of the $\text{su}_q(2)$ Spectrum

In this section we will consider some analytic expressions, which are based on the approximate result of Eq. (38), with the purpose of connecting the present approach to the Harris formalism [8]. In the study of high spin phenomena the rotational frequency ω and the kinematic moment of inertia \mathcal{J} are defined by

$$\hbar\omega = \frac{\partial E}{\partial \xi}, \quad (40)$$

$$\frac{\hbar^2}{2\mathcal{J}} = \frac{\partial E}{\partial \eta} = \frac{1}{2\xi} \frac{\partial E}{\partial \xi}, \quad (41)$$

where ξ and η have been defined in Eq. (37).

Applying these definitions to the analytical expression of Eq. (38) one can prove that the following expansions hold

$$E = \frac{A}{(2\tau)^2} \left((\omega t)^2 + \frac{1}{4}(\omega t)^4 + \frac{5}{8}(\omega t)^6 + \dots \right), \quad (42)$$

$$\xi = \sqrt{\ell(\ell+1)} = \frac{1}{2\tau} \left(\omega t + \frac{1}{6}(\omega t)^3 + \frac{3}{40}(\omega t)^5 + \frac{5}{112}(\omega t)^7 + \dots \right), \quad (43)$$

where

$$t = \frac{\hbar\tau}{A} = \frac{2\mathcal{J}_0}{\hbar} \tau \quad (44)$$

is a constant possessing dimensions of time.

The expansions appearing in Eqs. (42) and (43) are of the form occurring in the Harris formalism [8]

$$E = E_0 + \frac{1}{2}(\mathcal{J}_0\omega^2 + 3C\omega^4 + 5D\omega^6 + 7F\omega^8 + \dots), \quad (45)$$

$$\sqrt{\ell(\ell+1)} = \mathcal{J}_0\omega + 2C\omega^3 + 3D\omega^5 + 4F\omega^7 + \dots, \quad (46)$$

the main difference between the two formalisms being the fact that in the case of Harris the coefficients of the various terms in the series are independent from each other, while in the present case the coefficients in the series are interdependent, since they all contain the constant t . It should be noticed at this point that the Harris formalism is known [19] to be equivalent to the Variable Moment of Inertia (VMI) model [20]. The similarities between the $\text{su}_q(2)$ approach and the VMI model have been directly considered in Ref. [6].

7 Irreducible Tensor Operators under $\text{su}_q(2)$

A different path towards the construction of a Hamiltonian appropriate for the description of rotational spectra can be taken through the construction of irre-

ducible tensor operators (ITOs) under $\text{su}_q(2)$ [9, 10]. In this discussion we limit ourselves to real values of q , i.e. to $q = e^\tau$ with τ being real, as in Refs. [9, 10].

One can first construct an irreducible tensor operator of rank 1 under $\text{su}_q(2)$, using as building blocks the generators of $\text{su}_q(2)$. It turns out [9, 10, 21] that the explicit form of the relevant operators is

$$\begin{aligned} J_{+1} &= -\frac{1}{\sqrt{[2]}} q^{-L_0} L_+, & J_{-1} &= \frac{1}{\sqrt{[2]}} q^{-L_0} L_-, \\ J_0 &= \frac{1}{[2]} (q L_+ L_- - q^{-1} L_- L_+). \end{aligned} \quad (47)$$

It is clear that in the limit $q \rightarrow 1$ 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

$$J_+ = -\frac{L_x + iL_y}{\sqrt{2}}, \quad J_- = \frac{L_x - iL_y}{\sqrt{2}}, \quad J_0 = L_0. \quad (48)$$

One can also see that the operators

$$J'_m = \frac{J_m}{Z}, \quad m = +1, 0, -1, \quad (49)$$

where

$$Z = q^{-2L_0} + (q - q^{-1})J_0 = 1 + \frac{(q - q^{-1})^2}{[2]} C_2^{(q)}, \quad (50)$$

also form an irreducible tensor operator under $\text{su}_q(2)$.

One can now proceed with the construction of the scalar square of the angular momentum operator, a task which requires use of the scalar product of two ITOs [9, 10, 21–24], as well as use of the analytic expressions and symmetry properties of the q -deformed Clebsch–Gordan coefficients, which can be found in Refs. [9, 22]. In this way one finds the result

$$(J' \cdot J')^{(1/q)} = \frac{1 - Z^{-2}}{(q - q^{-1})^2}. \quad (51)$$

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

$$H = A \frac{1 - Z^{-2}}{(q - q^{-1})^2}, \quad (52)$$

where A is a constant, which we also write in the form

$$A = \frac{\hbar^2}{2\mathcal{J}_0} \quad (53)$$

for future reference.

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. (50), using the eigenvalues of the Casimir operator $C_2^{(q)}$ in this basis, which are $[\ell][\ell+1]$, as already mentioned in Section 2

$$\begin{aligned}\langle Z \rangle &= 1 + \frac{(q - q^{-1})^2}{[2]} [\ell][\ell + 1] = \frac{1}{[2]} (q^{2\ell+1} + q^{-2\ell-1}) \\ &= \frac{1}{[2]} ([2\ell + 2] - [2\ell]).\end{aligned}\quad (54)$$

Then the eigenvalues $\langle H \rangle$ of the Hamiltonian can be found by substituting the eigenvalues of Z from Eq. (54) into Eq. (52)

$$\begin{aligned}E = \langle H \rangle &= A \frac{1}{(q - q^{-1})^2} \left(1 - \frac{[2]^2}{(q^{2\ell+1} + q^{-2\ell-1})^2} \right) \\ &= A \frac{1}{4 \sinh^2 \tau} \left(1 - \frac{\cosh^2 \tau}{\cosh^2((2\ell + 1)\tau)} \right).\end{aligned}\quad (55)$$

From Eq. (54) it is clear that the eigenvalues of the scalar operator Z go to the limiting value 1 as $q \rightarrow 1$. Therefore one can think of Z as a “unity” operator. Furthermore the last expression in Eq. (54) indicates that $\langle Z \rangle$ is behaving like a “measure” of the unit of angular momentum in the deformed case.

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

For this purpose the notation and tools of Section 3 can be used once more. One can then prove that the Hamiltonian of Eq. (52) commutes with the generators \hat{l}_+ , \hat{l}_- , \hat{l}_0 of the usual $\text{su}(2)$ algebra, i.e. with the usual angular momentum operators

$$[\hat{H}, \hat{l}_+] |l, m\rangle_c = 0, \quad [\hat{H}, \hat{l}_-] |l, m\rangle_c = 0, \quad [\hat{H}, \hat{l}_0] |l, m\rangle_c = 0. \quad (56)$$

We have thus proved that the Hamiltonian of Eq. (52) is invariant under usual angular momentum. Therefore it should be possible to express the Hamiltonian itself as a function of \hat{C}_2 (the second order Casimir operator of $\text{su}(2)$). It should also be possible to express the eigenvalues of the Hamiltonian of Eq. (52) as a function of $l(l+1)$, i.e. as a function of the eigenvalues of \hat{C}_2 . This task will be undertaken in the following section.

9 Exact Expansion of the $\text{su}_q(2)$ ITO Spectrum

Since the Hamiltonian of Eq. (52) is invariant under $\text{su}(2)$, as we have seen in the last section, it should be possible to write its eigenvalues (given in Eq. (55)) as an expansion in terms of $l(l+1)$. This is a nontrivial task, since in Eq. (55)

a function of the variable ℓ appears, while we are in need of a function of the variable $\ell(\ell + 1)$, which is related to the length of the angular momentum vector.

It turns out that the spectrum of Eq. (55) can be put into the form

$$\frac{E}{A} = \left(\frac{\tau^2 \cosh^2 \tau}{\sinh^2 \tau} \right) \sum_{n=0}^{\infty} \frac{(-1)^n (2\tau)^n}{(n+1)!} f_n(\tau) (\ell(\ell+1))^{n+1}, \quad (57)$$

with

$$f_n(\tau) = (-1)^{n+1} (2\tau)^n (n+1)! \times \sum_{k=0}^{\infty} \frac{2^{2n+2k+4} (2^{2n+2k+4} - 1) B_{2n+2k+4}}{(2n+2k+2)!(2n+2k+4)} \binom{n+k+1}{n+1} \tau^{2k}, \quad (58)$$

where B_n are the Bernoulli numbers [18]. It is clear that Eq. (57) is an expansion in terms of $\ell(\ell + 1)$, as expected.

10 Approximate Expansion of the $\text{su}_q(2)$ ITO Spectrum

In the limit of $|\tau| \ll 1$ one is entitled to keep in Eq. (58) only the term with $k = 0$. Then one can prove that the relevant approximate form of the spectrum can be put into the compact form

$$E \approx \frac{A}{(2\tau)^2} \tanh^2(2\tau\sqrt{\ell(\ell+1)}) = \frac{A}{(2\tau)^2} \tanh^2(2\tau\xi), \quad (59)$$

where the notation of Eq. (37) is used again. The extended form of the Taylor expansion of E is then

$$E \approx A \left(\ell(\ell+1) - \frac{2}{3}(2\tau)^2(\ell(\ell+1))^2 + \frac{17}{45}(2\tau)^4(\ell(\ell+1))^3 - \frac{62}{315}(2\tau)^6(\ell(\ell+1))^4 + \dots \right). \quad (60)$$

Eq. (59) will be referred to as the ‘‘hyperbolic tangent formula’’.

11 Analytic Expressions Based on the Approximate Expansion of the $\text{su}_q(2)$ ITO Spectrum

We are now going to derive analytic formulae for the rotational frequency ω and the kinematic moment of inertia \mathcal{J} , based on the approximate expression for the energy given in Eq. (59). Using Eqs. (40) and (41) one obtains the following expansions in terms of powers of ω^2

$$E = \frac{A}{(2\tau)^2} ((\omega t)^2 + 2(\omega t)^4 + 7(\omega t)^6 + 30(\omega t)^8 + 143(\omega t)^{10} + \dots), \quad (61)$$

$$\xi = \sqrt{\ell(\ell + 1)} = \frac{\mathcal{J}_0}{\hbar} \omega \left(1 + \frac{4}{3}(\omega t)^2 + \frac{21}{5}(\omega t)^4 + \frac{120}{7}(\omega t)^6 + \frac{715}{9}(\omega t)^8 + \frac{4368}{11}(\omega t)^{10} + \dots \right), \quad (62)$$

where the constant t of Eq. (44) appears once more. Eqs. (61) and (62) give the energy and the quantity $\sqrt{\ell(\ell + 1)}$ as series in powers of the rotational frequency ω , thus making contact between the present approach and the Harris formalism [8], given in Eqs. (45) and (46).

12 Numerical Tests

The formulae developed in the previous sections have been tested against the experimental spectra of the Th isotopes [25–29], which range from vibrational (^{222}Th with $R_4 = E(4)/E(2) = 2.399$) to clearly rotational (^{234}Th with $R_4 = 3.308$). The purpose of this study is two-fold:

- a) To test the quality of the approximations used in Sections 5 and 10.
- b) To test the agreement between theoretical predictions and experimental data.

The standard rotational expansion,

$$E = A\ell(\ell + 1) + B(\ell(\ell + 1))^2 + C(\ell(\ell + 1))^3 + D(\ell(\ell + 1))^4 + \dots, \quad (63)$$

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 [11]

$$E = a(\sqrt{1 + b\ell(\ell + 1)} - 1), \quad (64)$$

which is known to give the best fits to experimental rotational nuclear spectra among all two-parameter expressions [12], will be included in the test for comparison. For brevity we are going to use the following terminology:

- Model I for Eq. (15) (original $\text{su}_q(2)$ formula),
- Model I' for Eq. (38) (“the sinus formula”),
- Model II for Eq. (55) (“the $\text{su}_q(2)$ irreducible tensor operator (ITO) formula”),
- Model II' for Eq. (59) (“the hyperbolic tangent formula”),
- Model III for Eq. (63) (the standard rotational formula), and
- Model IV for Eq. (64) (the Holmberg–Lipas formula).

The standard quality measure

$$\sigma = \sqrt{\frac{2}{\ell_{max}} \sum_{i=2}^{\ell_{max}} (E_{exp}(\ell) - E_{th}(\ell))^2}, \quad (65)$$

where ℓ_{max} is the angular momentum of the highest level included in the fit, has been used for judging the quality of the fits.

From the results of these fits the following observations can be made:

a) 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 Sections 5 and 10 are very accurate.

b) All models give good results for ^{226}Th - ^{234}Th , which lie in the rotational region, with R_4 ratio between 3.136 and 3.308, with model IV giving the best results and model III giving the worst ones, while in all cases models II and II' are better than models I and I'. It should be noticed, however, that all models tend to underestimate the first several levels of the spectra and the last one or two levels, while they overestimate the rest of the levels. In other words, all models "fail in the same way".

c) A similar picture holds for the transitional nucleus ^{224}Th ($R_4 = 2.896$) and the near-vibrational nucleus ^{222}Th ($R_4 = 2.399$), i.e. still model IV gives the best results and model III the worst, while models II and II' are better than models I and I'. However, the deviations from the data get much larger, indicating that all these models are inappropriate for describing spectra in the vibrational and transitional regions, in which the presence of a term linear in ℓ is required, as in the u(5) and o(6) limits of the Interacting Boson Model [30].

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, the rotational frequency and the moment of inertia.

b) The fact that models II and II' are better than models I and I' indicates that within the same symmetry ($\text{su}_q(2)$ in this case) it is possible to construct different rotational Hamiltonians characterized by different degrees of agreement with the data. However, these Hamiltonians are too "rigid", in the sense that they can describe only rotational spectra, while vibrational and transitional spectra are outside their realm.

13 Discussion

The main results of the present work are the following:

a) The rotational invariance of the original $\text{su}_q(2)$ Hamiltonian [5,6] under the usual physical angular momentum has been proved explicitly and its connections to the formalisms of Amal'sky [7] ("the sinus formula") and Harris [8] have been given.

b) An irreducible tensor operator (ITO) of rank one under $\text{su}_q(2)$ has been found and used, through q -deformed tensor product and q -deformed Clebsch-Gordan coefficient techniques [9,10,22,23], for the construction of a new Hamiltonian appropriate for the description of rotational spectra, the $\text{su}_q(2)$ ITO Hamil-

tonian. The rotational invariance of this new Hamiltonian under the usual physical angular momentum has been proved explicitly. Furthermore, an approximate simple closed expression (“the hyperbolic tangent formula”) for the energy spectrum of this Hamiltonian has been found and its connection to the Harris [8] formalism has been demonstrated.

From the results of the present work it is clear that the $su_q(2)$ Hamiltonian, as well as the $su_q(2)$ ITO Hamiltonian, are complicated functions of the Casimir operator of the usual $su(2)$, i.e. of the square of the usual physical angular momentum. These complicated functions possess the $su_q(2)$ symmetry, in addition to the usual $su(2)$ 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. This operator would allow the study of multi-band spectra, in analogy to the Elliott model [31], as well as the study of BE(2) transition probabilities. Since q -deformation appears to describe well the stretching effect of rotational nuclear spectra, it is interesting to check what its influence on the corresponding B(E2) transition probabilities will be. Work in this direction is in progress.

It should be noticed that the $su_q(2)$ ITO techniques used above can also be applied to the description of magic numbers and supershells in metal clusters (see Refs. [32, 33] for relevant details).

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