QUANTUM ALGEBRAIC SYMMETRIES
IN NUCLEI, MOLECULES, AND ATOMIC CLUSTERS

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Abstract

Various applications of quantum algebraic techniques in nuclear structure physics and in molecular physics are briefly reviewed and a recent application of these techniques to the structure of atomic clusters is discussed in more detail.

1. Introduction

Quantum algebras (also called quantum groups) [1, 2, 3] are deformed versions of the usual Lie algebras, to which they reduce when the deformation parameter $q$ is set equal to unity. From the mathematical point of view they are Hopf algebras. Their use in physics became popular with the introduction [4, 5] of the $q$-deformed harmonic oscillator as a tool for providing a boson realization of the quantum algebra $su_q(2)$, although similar mathematical structures had already been known [6]. Initially used for solving the quantum Yang–Baxter equation, quantum algebras have subsequently found applications in several branches of physics, as, for example, in the description of spin chains, squeezed states [7], hydrogen atom and hydrogen-like spectra [8, 9, 10], rotational and vibrational nuclear and molecular spectra and in conformal field theories. By now much work has been done [11, 12, 13, 14] on the $q$-deformed oscillator and its relativistic extensions [15, 16], and several kinds of generalized deformed oscillators [17, 18, 19, 20] and generalized deformed $su(2)$ algebras [21, 22, 23, 24] have been introduced.

Here we shall confine ourselves to applications of quantum algebras in nuclear structure physics and in molecular physics. The purpose of this short review is to provide the reader with references for further reading. In addition a recent application of quantum algebraic techniques to the structure of atomic clusters will be discussed in more detail.

2. The $su_q(2)$ rotator model

The first application of quantum algebras in nuclear physics was the use of the deformed algebra $su_q(2)$ for the description of the rotational spectra of deformed [25, 26] and superdeformed [27] nuclei. The Hamiltonian of the $q$-deformed rotator is proportional to the second order Casimir operator of the $su_q(2)$ algebra. Its Taylor expansion contains powers of $J(J+1)$ (where $J$ is the angular momentum), being similar [26] to the expansion provided by the Variable Moment of Inertia (VMI) model. Furthermore, the deformation parameter $\tau$ (with $q = e^{i\tau}$) has been found [26] to correspond to the softness parameter of the VMI model. Through a comparison of the $su_q(2)$ model to the hybrid model the deformation parameter $\tau$ has also been connected to the number of valence nucleon pairs [28] and to the nuclear deformation $\beta$ [29]. Since $\tau$ is an indicator of deviation from the
pure su(2) symmetry, it is not surprising that $\tau$ decreases with increasing $\beta$ \[29\]. The su$_q$(2) model has been recently extended to excited (beta and gamma) bands \[30\].

B(E2) transition probabilities have also been described in this framework \[31\]. In this case the $q$-deformed Clebsch–Gordan coefficients are used instead of the normal ones. (It should be noticed that the $q$-deformed angular momentum theory has already been much developed \[31\].) The model predicts an increase of the B(E2) values with angular momentum, while the rigid rotator model predicts saturation. Some experimental results supporting this prediction already exist \[31\]. Similarly increasing B(E2) values are predicted by a modified version \[32\] of the su(3) limit of the Interacting Boson Model (IBM), by the su(3) limit of the sdg Interacting Boson Model \[33\], by the Fermion Dynamical Symmetry Model (FDSM) \[34\], as well as by the recent systematics of Zamfir and Casten \[35\].

3. Extensions of the su$_q$(2) model

The su$_q$(2) model has been successful in describing rotational nuclear spectra. For the description of vibrational and transitional nuclear spectra it has been found \[36\] that $J(J + 1)$ has to be replaced by $J(J + c)$. The additional parameter $c$ allows for the description of nuclear anharmonicities in a way similar to that of the Interacting Boson Model (IBM) and the Generalized Variable Moment of Inertia (GVMI) model \[37\]. The use of $J(J + c)$ instead of $J(J + 1)$ for vibrational and transitional nuclei is also supported by recent systematics \[38\].

Another generalization is based on the use of the deformed algebra su$_\Phi$(2) \[21, 22, 23, 24\], which is characterized by a structure function $\Phi$. The usual su(2) and su$_q$(2) algebras are obtained for specific choices of the structure function $\Phi$. The su$_\Phi$(2) algebra has been constructed so that its representation theory resembles as much as possible the representation theory of the usual su(2) algebra. Using this technique one can construct, for example, a rotator having the same spectrum as the one given by the Holmberg–Lipas formula \[39\]. A two-parameter generalization of the su$_q$(2) model, labelled as su$_{qp}$(2), has also been successfully used for the description of superdeformed nuclear bands \[40\].

4. Pairing correlations

It has been found \[41\] that correlated fermion pairs coupled to zero angular momentum in a single-$j$ shell behave approximately as suitably defined $q$-deformed bosons. After performing the same boson mapping to a simple pairing Hamiltonian, one sees that the pairing energies are also correctly reproduced up to the same order. The deformation parameter used ($\tau = \ln q$) is found to be inversely proportional to the size of the shell, thus serving as a small parameter.

The above mentioned system of correlated fermion pairs can be described exactly by suitably defined generalized deformed bosons \[42\]. Then both the commutation relations are satisfied exactly and the pairing energies are reproduced exactly. The spectrum of the appropriate generalized deformed oscillator corresponds, up to first order perturbation theory, to a harmonic oscillator with an $x^4$ perturbation.

If one considers, in addition to the pairs coupled to zero angular momentum, pairs coupled to non-zero angular momenta, one finds that an approximate description in terms of
two suitably defined \( q \)-oscillators (one describing the \( J = 0 \) pairs and the other corresponding to the \( J \neq 0 \) pairs) occurs [43]. The additional terms introduced by the deformation have been found [43] to improve the description of the neutron pair separation energies of the Sn isotopes, with no extra parameter introduced.

\( q \)-deformed versions of the pairing theory have also been given in [44, 45].

5. \( q \)-deformed versions of nuclear models

A \( q \)-deformed version of a two dimensional toy Interacting Boson Model (IBM) with \( \text{su}_q(3) \) overall symmetry has been developed [46, 47], mainly for testing the ways in which spectra and transition probabilities are influenced by the \( q \)-deformation. The question of possible complete breaking of the symmetry through \( q \)-deformation, i.e. the transition from the \( \text{su}_q(2) \) limiting symmetry to the \( \text{so}_q(3) \) one has been examined [48, 49]. It has been found that such a transition is possible for complex values of the parameter \( q \) [49]. (For problems arising when using complex \( q \) values see [50]). Complete breaking of the symmetry has also been considered in the framework of an \( \text{su}_q(2) \) model [51]. It has also been found [52] that \( q \)-deformation leads (for specific range of values of the deformation parameter \( \tau \), with \( q = e^{i\tau} \)) to a recovery of the \( u(3) \) symmetry in the framework of a simple Nilsson model including a spin-orbit term. Finally, the \( \text{so}_q(3) \) limit of the toy IBM model has been used for the description of \( ^{16}\text{O} + \alpha \) cluster states in \( ^{20}\text{Ne} \), with positive results [53].

\( q \)-deformed versions of the \( \text{o}(6) \) and \( \text{u}(5) \) limits of the full IBM have been discussed in [54, 55, 56]. The \( q \)-deformation of the \( \text{su}(3) \) limit of IBM is a formidable problem, since the \( \text{su}_q(3) \supset \text{so}_q(3) \) decomposition has for the moment been achieved only for completely symmetric \( \text{su}_q(3) \) irreducible representations [57, 58, 59].

Furthermore a \( q \)-deformed version of the Moszkowski model has been developed [60, 61] and RPA modes have been studied [62] in it. A \( q \)-deformed Moszkowski model with cranking has also been studied [63] in the mean-field approximation. It has been seen that the residual interaction simulated by the \( q \)-deformation is felt more strongly by states with large \( J_\pi \). The possibility of using \( q \)-deformation in assimilating temperature effects is receiving attention, since it has also been found [64] that this approach can be used in describing thermal effects in the framework of a \( q \)-deformed Thouless model for superconductivity.

In addition, \( q \)-deformed versions of the Lipkin-Meshkov-Glick (LMG) model have been developed, both for the 2-level version of the model in terms of an \( \text{su}_q(2) \) algebra [65], and for the 3-level version of the model in terms of an \( \text{su}_q(3) \) algebra [66].

6. Anisotropic quantum harmonic oscillator with rational ratios of frequencies

The symmetries of the 3-dimensional anisotropic quantum harmonic oscillator with rational ratios of frequencies (RHO) are of high current interest in nuclear physics, since they are the basic symmetries underlying the structure of superdeformed and hyperdeformed nuclei [67, 68]. The 2-dimensional RHO is also of interest, in connection with “pancake” nuclei [69], i.e. very oblate nuclei. Cluster configurations in light nuclei can also be described [70] in terms of RHO symmetries, which underlie the geometrical structure of the Bloch–Brink \( \alpha \)-cluster model [71]. The 3-dim RHO is also of interest for the interpretation of the
observed shell structure in atomic clusters [72, 73], especially after the realization that large deformations can occur in such systems [74]. (See section 9 for further discussion of atomic clusters.)

The two-dimensional and three-dimensional [75] anisotropic harmonic oscillators have been the subject of several investigations, both at the classical and the quantum mechanical level (see [76, 77] for references). These oscillators are examples of superintegrable systems. The special cases with frequency ratios 1:2 and 1:3 have also been considered [78]. While at the classical level it is clear that the su(N) or sp(2N,R) algebras can be used for the description of the N-dimensional anisotropic oscillator, the situation at the quantum level, even in the two-dimensional case, is not as simple. It has been proved that a generalized deformed u(2) algebra is the symmetry algebra of the two-dimensional anisotropic quantum harmonic oscillator [76], which is the oscillator describing the single-particle level spectrum of “pancake” nuclei, i.e. of triaxially deformed nuclei with $\omega_x >> \omega_y, \omega_z$. Furthermore, a generalized deformed u(3) algebra turns out to be the symmetry algebra of the three-dimensional RHO [77].

7. Three-dimensional $q$-deformed (isotropic) harmonic oscillator

Recently the 3-dimensional $q$-deformed (isotropic) harmonic oscillator has been studied in detail [79], following the mathematical developments of [57, 58, 59]. It turns out that in this framework, one can reproduce level schemes similar to the ones occurring in the modified harmonic oscillator model, first suggested by Nilsson [80, 81]. An appropriate $q$-deformed spin–orbit interaction term has also been developed [79]. Including this term in the 3-dimensional $q$-deformed (isotropic) harmonic oscillator scheme one can reproduce level schemes similar to these provided by the modified harmonic oscillator with spin–orbit interaction. It is expected that this scheme, without the spin–orbit interaction term, will be appropriate for describing the magic numbers occurring in the various kinds of atomic clusters [72, 73], since a description of magic numbers of atomic clusters in terms of a Nilsson model without a spin–orbit interaction has already been attempted [82]. This subject will be discussed in some detail in Section 9.

A recent review of the applications of quantum algebraic techniques to nuclear structure problems can be found in [83].

8. The use of quantum algebras in molecular structure

Similar techniques can be applied in describing properties of diatomic and polyatomic molecules. A brief list will be given here.

1) Rotational spectra of diatomic molecules have been described in terms of the $su_q(2)$ model [84]. As in the case of nuclei, $q$ is a phase factor ($q = e^{i\tau}$). In molecules $\tau$ is of the order of 0.01. The use of the $su_q(2)$ symmetry leads to a partial summation of the Dunham expansion describing the rotational–vibrational spectra of diatomic molecules [84]. Molecular backbending (bandcrossing) has also been described in this framework [83]. Rotational spectra of symmetric top molecules have also been considered [86, 87] in the framework of the $su_q(2)$ symmetry. Furthermore, two $q$-deformed rotators with slightly different parameter values have been used [88] for the description of $\Delta I = 1$ staggering
effects in rotational bands of diatomic molecules. (For a discussion of \( \Delta I = 2 \) staggering effects in diatomic molecules see \[89\]).

2) Vibrational spectra of diatomic molecules have been described in terms of \( q \)-deformed anharmonic oscillators having the \( \text{su}(1,1) \) \[90\] or the \( \text{so}_q(2) \) \[91\] symmetry, as well as in terms of generalized deformed oscillators similar to the ones described in sec. 3 \[92, 93\]. These results, combined with 1), lead to the full summation of the Dunham expansion \[90, 91\]. A two-parameter deformed anharmonic oscillator with \( \text{u}_{qp}(2) \supset \text{o}_{qp}(2) \) symmetry has also been considered \[94\].

3) The physical content of the anharmonic oscillators mentioned in 2) has been clarified by constructing WKB equivalent potentials (WKB-EPs) and classical equivalent potentials \[95\] providing approximately the same spectrum. The results have been corroborated by the study of the relation between \( \text{su}_q(1,1) \) and the anharmonic oscillator with \( x^4 \) anharmonicities \[96\]. Furthermore the WKB-EP corresponding to the \( \text{su}_q(1,1) \) anharmonic oscillator has been connected to a class of Quasi-Exactly Soluble Potentials (QESPs) \[97\].

4) Generalized deformed oscillators giving the same spectrum as the Morse potential \[98\] and the modified Pöschl–Teller potential \[99\], as well as a deformed oscillator containing them as special cases \[100\] have also been constructed. In addition, \( q \)-deformed versions of the Morse potential have been given, either by using the \( \text{so}_q(2,1) \) symmetry \[101\] or by solving a \( q \)-deformed Schrödinger equation for the usual Morse potential \[102\]. For the sake of completeness it should be mentioned that a deformed oscillator giving the same spectrum as the Coulomb potential has also been constructed \[103\].

5) A \( q \)-deformed version of the vibron model for diatomic molecules has been constructed \[104\], in a way similar to that described in sec. 5.

6) For vibrational spectra of polyatomic molecules a model of \( n \) coupled generalized deformed oscillators has been built \[105\], containing the approach of Iachello and Oss \[106\] as a special case. In addition a model of two \( Q \)-deformed oscillators coupled so that the total Hamiltonian has the \( \text{su}_Q(2) \) symmetry has been proved \[107\] to be equivalent, to lowest order approximation, to a system of two identical Morse oscillators coupled by the cross-anharmonicity usually used empirically in describing vibrational spectra of diatomic molecules.

7) Quasi-molecular resonances in the systems \( ^{12}\text{C}^+^{12}\text{C} \) and \( ^{12}\text{C}^+^{16}\text{O} \) have been described in terms of a \( q \)-deformed oscillator plus a rigid rotator \[108\].

A review of several of the above topics, concerning the applications of quantum algebraic techniques to molecular structure, accompanied by a detailed and self-contained introduction to quantum algebras, has been given by Raychev \[109\].

9. The 3-dimensional \( q \)-deformed harmonic oscillator and magic numbers of alkali metal clusters

Metal clusters have been recently the subject of many investigations (see \[72, 73, 110\] for relevant reviews). One of the first fascinating findings in their study was the appearance of magic numbers \[111, 112, 113, 114, 115, 116, 117\], analogous to but different from the magic numbers appearing in the shell structure of atomic nuclei \[118\]. This analogy led to the early description of metal clusters in terms of the Nilsson–Clemenger model \[82\].
which is a simplified version of the Nilsson model \[80, 81\] of atomic nuclei, in which no spin-orbit interaction is included. Further theoretical investigations in terms of the jellium model \[119, 120\] demonstrated that the mean field potential in the case of simple metal clusters bears great similarities to the Woods–Saxon potential of atomic nuclei, with a slight modification of the “wine bottle” type \[121\]. The Woods–Saxon potential itself looks like a harmonic oscillator truncated at a certain energy value and flattened at the bottom. It should also be recalled that an early schematic explanation of the magic numbers of metallic clusters has been given in terms of a scheme intermediate between the level scheme of the 3-dimensional harmonic oscillator and the square well \[72\]. Again in this case the intermediate potential resembles a harmonic oscillator flattened at the bottom.

On the other hand, modified versions of harmonic oscillators \[4, 5\] have been recently investigated, as it has already been mentioned. The spectra of $q$-deformed oscillators increase either less rapidly (for $q$ being a phase factor, i.e. $q = e^{i\tau}$ with $\tau$ being real) or more rapidly (for $q$ being real, i.e. $q = e^{\tau}$ with $\tau$ being real) in comparison to the equidistant spectrum of the usual harmonic oscillator \[83\], while the corresponding (WKB-equivalent) potentials \[83\] resemble the harmonic oscillator potential, truncated at a certain energy (for $q$ being a phase factor) or not (for $q$ being real), the deformation inflicting an overall widening or narrowing of the potential, depending on the value of the deformation parameter $q$.

Very recently, a $q$-deformed version of the 3-dimensional harmonic oscillator has been constructed \[79\], taking advantage of the $u_q(3) \supset so_q(3)$ symmetry \[122, 79\]. As it has already been mentioned in Section 7, the spectrum of this 3-dimensional $q$-deformed harmonic oscillator has been found \[79\] to reproduce very well the spectrum of the modified harmonic oscillator introduced by Nilsson \[80, 81\], without the spin-orbit interaction term. Since the Nilsson model without the spin-orbit term is essentially the Nilsson–Clemenger model used for the description of metallic clusters \[82\], it is worth examining if the 3-dimensional $q$-deformed harmonic oscillator can reproduce the magic numbers of simple metallic clusters. This is the subject of the present section.

The space of the 3-dimensional $q$-deformed harmonic oscillator consists of the completely symmetric irreducible representations of the quantum algebra $u_q(3)$. In this space a deformed angular momentum algebra, $so_q(3)$, can be defined \[79\]. The Hamiltonian of the 3-dimensional $q$-deformed harmonic oscillator is defined so that it satisfies the following requirements:

a) It is an $so_q(3)$ scalar, i.e. the energy is simultaneously measurable with the $q$-deformed angular momentum related to the algebra $so_q(3)$ and its z-projection.

b) It conserves the number of bosons, in terms of which the quantum algebras $u_q(3)$ and $so_q(3)$ are realized.

c) In the limit $q \to 1$ it is in agreement with the Hamiltonian of the usual 3-dimensional harmonic oscillator.

It has been proved \[79\] that the Hamiltonian of the 3-dimensional $q$-deformed harmonic oscillator satisfying the above requirements takes the form

$$H_q = \hbar \omega_0 \left\{ |N| q^{N+1} - \frac{q(q - q^{-1})}{[2]} C_q^{(2)} \right\},$$

where $N$ is the number operator and $C_q^{(2)}$ is the second order Casimir operator of the algebra.
so \( q(3) \), while

\[
[x] = \frac{q^x - q^{-x}}{q - q^{-1}}
\]

is the definition of \( q \)-numbers and \( q \)-operators.

The energy eigenvalues of the 3-dimensional \( q \)-deformed harmonic oscillator are then

\[
E_q(n, l) = \hbar \omega_0 \left\{ [n]q^{n+1} - \frac{q(q - q^{-1})}{[2]}[l][l + 1] \right\},
\]

where \( n \) is the number of vibrational quanta and \( l \) is the eigenvalue of the angular momentum, obtaining the values \( l = n, n - 2, \ldots, 0 \) or 1.

In the limit of \( q \to 1 \) one obtains \( \lim_{q \to 1} E_q(n, l) = \hbar \omega_0 n \), which coincides with the classical result.

For small values of the deformation parameter \( \tau \) (where \( q = e^\tau \)) one can expand eq. (3) in powers of \( \tau \) obtaining

\[
E_q(n, l) = \hbar \omega_0 n - \hbar \omega_0 \tau (l(l+1) - n(n+1))
- \hbar \omega_0 \tau^2 \left( l(l+1) - \frac{1}{3} n(n+1)(2n+1) \right) + \mathcal{O}(\tau^3).
\]

The last expression to leading order bears great similarity to the modified harmonic oscillator suggested by Nilsson [80, 81] (with the spin-orbit term omitted)

\[
V = \frac{1}{2} \hbar \omega \rho^2 - \hbar \omega \kappa' (L^2 - <L^2>_N), \quad \rho = r \sqrt{\frac{M \omega}{\hbar}},
\]

where

\[
<L^2>_N = \frac{N(N+3)}{2}.
\]

It has been proved [79] that the spectrum of the 3-dimensional \( q \)-deformed harmonic oscillator closely reproduces the spectrum of the modified harmonic oscillator of Nilsson. In both cases the effect of the \( l(l+1) \) term is to flatten the bottom of the harmonic oscillator potential, thus making it to resemble the Woods–Saxon potential.

The level scheme of the 3-dimensional \( q \)-deformed harmonic oscillator (for \( \hbar \omega_0 = 1 \) and \( \tau = 0.038 \)) is given in Table 1 [123], up to a certain energy. Each level is characterized by the quantum numbers \( n \) (number of vibrational quanta) and \( l \) (angular momentum). Next to each level its energy, the number of particles it can accommodate (which is equal to \( 2(2l+1) \)) and the total number of particles up to and including this level are given. If the energy difference between two successive levels is larger than 0.39, it is considered as a gap separating two successive shells and the energy difference is reported between the two levels. In this way magic numbers can be easily read in the table: they are the numbers appearing above the gaps, written in boldface characters.

The magic numbers provided by the 3-dimensional \( q \)-deformed harmonic oscillator in Table 1 are compared to available experimental data for Na clusters [111, 112, 113, 115, 116] in Table 2 (columns 2–6) [123]. The following comments apply:
i) Only magic numbers up to 1500 are reported, since it is known that filling of electronic shells is expected to occur only up to this limit \[111\]. For large clusters beyond this point it is known that magic numbers can be explained by the completion of icosahedral or cuboctahedral shells of atoms \[111\].

ii) Up to 600 particles there is consistency among the various experiments and between the experimental results in one hand and our findings in the other.

iii) Beyond 600 particles the predictions of the three experiments, which report magic numbers in this region, are quite different. However, the predictions of all three experiments are well accommodated by the present model. Magic numbers 694, 832, 1012 are supported by the findings of both Martin et al. \[111\] and Bréchignac et al. \[116\], magic numbers 1206, 1410 are in agreement with the experimental findings of Martin et al. \[111\], magic numbers 912, 1284 are supported by the findings of Bréchignac et al., while magic numbers 676, 1100, 1314, 1502 are in agreement with the experimental findings of Pedersen et al. \[115\].

In Table 2 the predictions of three simple theoretical models \[118\] (non-deformed 3-dimensional harmonic oscillator (column 9), square well potential (column 8), rounded square well potential (intermediate between the previous two, column 7) ) are also reported for comparison. It is clear that the predictions of the non-deformed 3-dimensional harmonic oscillator are in agreement with the experimental data only up to magic number 40, while the other two models give correctly a few more magic numbers (58, 92, 138), although they already fail by predicting magic numbers at 68, 70, 106, 112, 156, which are not observed.

It should be noticed at this point that the first few magic numbers of alkali clusters (up to 92) can be correctly reproduced by the assumption of the formation of shells of atoms instead of shells of delocalized electrons \[124\], this assumption being applicable under conditions not favoring delocalization of the valence electrons of alkali atoms.

Comparisons among the present results, experimental data (by Martin et al. \[111\] (column 2), Pedersen et al. \[115\] (column 3) and Bréchignac et al. \[116\] (column 4) ) and theoretical predictions more sophisticated than those reported in Table 2, can be made in Table 3 \[123\], where magic numbers predicted by various jellium model calculations (columns 5–8, \[111\] \[112\] \[73\] \[74\] ), Woods–Saxon and wine bottle potentials (column 9, \[125\]), as well as by a classification scheme using the $3n + l$ pseudo quantum number (column 10, \[111\] ) are reported. The following observations can be made:

i) All magic numbers predicted by the 3-dimensional $q$-deformed harmonic oscillator are supported by at least one experiment, with no exception.

ii) Some of the jellium models, as well as the $3n + l$ classification scheme, predict magic numbers at 186, 540/542, which are not supported by experiment. Some jellium models also predict a magic number at 748 or 758, again without support from experiment. The Woods–Saxon and wine bottle potentials of Ref. \[123\] predict a magic number at 68, for which no experimental support exists. The present scheme avoids problems at these numbers. It should be noticed, however, that in the cases of 186 and 542 the energy gap following them in the present scheme is 0.329 and 0.325 respectively (see Table 1), i.e. quite close to the threshold of 0.39 which we have considered as the minimum energy gap separating different shells. One could therefore qualitatively remark that 186 and 542 are
“built in” the present scheme as “secondary” (not very pronounced) magic numbers.

The following general remarks can also be made:

i) It is quite remarkable that the 3-dimensional $q$-deformed harmonic oscillator reproduces the magic numbers at least as accurately as other, more sophisticated, models by using only one free parameter ($q = e^7$). Once the parameter is fixed, the whole spectrum is fixed and no further manipulations can be made. This can be considered as evidence that the 3-dimensional $q$-deformed harmonic oscillator owns a symmetry (the $u_q(3) \supset so_q(3)$ symmetry) appropriate for the description of the physical systems under study.

ii) It has been remarked [11] that if $n$ is the number of nodes in the solution of the radial Schrödinger equation and $l$ is the angular momentum quantum number, then the degeneracy of energy levels of the hydrogen atom characterized by the same $n + l$ is due to the $so(4)$ symmetry of this system, while the degeneracy of energy levels of the spherical harmonic oscillator (i.e. of the 3-dimensional isotropic harmonic oscillator) characterized by the same $2n + l$ is due to the $su(3)$ symmetry of this system. $3n + l$ has been used [11] to approximate the magic numbers of alkali metal clusters with some success, but no relevant Lie symmetry could be determined. In view of the present findings the lack of Lie symmetry related to $3n + l$ is quite clear: the symmetry of the system appears to be a quantum algebraic symmetry ($u_q(3)$), which is a nonlinear extension of the Lie symmetry $u(3)$.

iii) An interesting problem is to determine a WKB-equivalent potential giving (within this approximation) the same spectrum as the 3-dimensional $q$-deformed harmonic oscillator, using methods similar to these of Ref. [9]. The similarity between the results of the present model and those provided by the Woods–Saxon potential (column 9 in Table 3) suggests that the answer should be a harmonic oscillator potential flattened at the bottom, similar to the Woods–Saxon potential. If such a WKB-equivalent potential will show any similarity to a wine bottle shape, as several potentials used for the description of metal clusters do [19, 20, 21], remains to be seen.

In summary, we have shown in this section that the 3-dimensional $q$-deformed harmonic oscillator with $u_q(3) \supset so_q(3)$ symmetry correctly predicts all experimentally observed magic numbers of alkali metal clusters up to 1500, which is the expected limit of validity for theories based on the filling of electronic shells. This indicates that $u_q(3)$, which is a nonlinear deformation of the $u(3)$ symmetry of the spherical (3-dimensional isotropic) harmonic oscillator, is a good candidate for being the symmetry of systems of alkali metal clusters.

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Table 1: Energy spectrum, $E_q(n, l)$, of the 3-dimensional $q$-deformed harmonic oscillator (eq. (3)), for $\hbar \omega_0 = 1$ and $q = e^\tau$ with $\tau = 0.038$. Each level is characterized by $n$ (the number of vibrational quanta) and $l$ (the angular momentum). $2(2l + 1)$ represents the number of particles each level can accommodate, while under “total” the total number of particles up to and including this level is given. Magic numbers, reported in boldface, correspond to energy gaps larger than 0.39, reported between the relevant couples of energy levels.

| $n$ | $l$ | $E_q(n, l)$ | $2(2l + 1)$ | total | $n$ | $l$ | $E_q(n, l)$ | $2(2l + 1)$ | total |
|-----|-----|-------------|-------------|-------|-----|-----|-------------|-------------|-------|
| 0   | 0   | 0.000       | 2           | 2     | 9   | 5   | 12.215      | 22          | 462   |
|     |     | 1.000       |             |       | 11  | 11  | 12.315      | 46          | 508   |
| 1   | 1   | 1.000       | 6           | 8     | 10  | 8   | 12.614      | 34          | 542   |
|     |     | 1.006       |             |       | 9   | 3   | 12.939      | 14          | 556   |
| 2   | 2   | 2.006       | 10          | 18    |     |     |             |             |       |
| 2   | 0   | 2.243       | 2           | 20    | 9   | 1   | 13.336      | 6           | 562   |
|     |     | 0.780       |             |       | 12  | 12  | 13.721      | 50          | 612   |
| 3   | 3   | 3.023       | 14          | 34    | 10  | 6   | 13.863      | 26          | 638   |
|     |     | 0.397       |             |       | 11  | 9   | 14.154      | 38          | 676   |
| 3   | 1   | 3.420       | 6           | 40    |     |     |             |             |       |
|     |     | 0.638       |             |       | 10  | 4   | 14.757      | 18          | 694   |
| 4   | 4   | 4.058       | 18          | 58    |     |     |             |             |       |
|     |     | 0.559       |             |       | 13  | 13  | 15.206      | 54          | 748   |
| 4   | 2   | 4.617       | 10          | 68    | 10  | 2   | 15.316      | 10          | 758   |
| 4   | 0   | 4.854       | 2           | 70    | 10  | 0   | 15.554      | 2           | 760   |
| 5   | 5   | 5.116       | 22          | 92    | 11  | 7   | 15.592      | 30          | 790   |
|     |     | 0.724       |             |       | 12  | 10  | 15.777      | 42          | 832   |
| 5   | 3   | 5.841       | 14          | 106   |     |     |             |             |       |
| 6   | 6   | 6.204       | 26          | 132   | 11  | 5   | 16.660      | 22          | 854   |
| 5   | 1   | 6.238       | 6           | 138   | 14  | 14  | 16.779      | 58          | 912   |
|     |     | 0.860       |             |       | 0.606|     |             |             |       |
| 6   | 4   | 7.098       | 18          | 156   | 11  | 3   | 17.385      | 14          | 926   |
| 7   | 7   | 7.328       | 30          | 186   | 12  | 8   | 17.410      | 34          | 960   |
| 6   | 2   | 7.657       | 10          | 196   | 13  | 11  | 17.490      | 46          | 1006  |
| 6   | 0   | 7.895       | 2           | 198   | 11  | 1   | 17.782      | 6           | 1012  |
|     |     | 0.502       |             |       | 0.667|     |             |             |       |
| 7   | 5   | 8.396       | 22          | 220   | 15  | 15  | 18.449      | 62          | 1074  |
| 8   | 8   | 8.494       | 34          | 254   | 12  | 6   | 18.660      | 26          | 1100  |
|     |     | 0.627       |             |       | 0.645|     |             |             |       |
| 7   | 3   | 9.121       | 14          | 268   | 14  | 12  | 19.305      | 50          | 1150  |
|     |     | 0.397       |             |       | 13  | 9   | 19.330      | 38          | 1188  |
| 7   | 1   | 9.518       | 6           | 274   | 12  | 4   | 19.554      | 18          | 1206  |
| 9   | 9   | 9.709       | 38          | 312   |     |     |             |             |       |
| 8   | 6   | 9.743       | 26          | 338   | 12  | 2   | 20.113      | 10          | 1216  |
|     |     | 0.894       |             |       | 16  | 16  | 20.226      | 66          | 1282  |
| 8   | 4   | 10.637      | 18          | 356   | 12  | 0   | 20.350      | 2           | 1284  |
| 10  | 10  | 10.980      | 42          | 398   | 17  |     |             |             | 0.417 |
| 9   | 7   | 11.146      | 30          | 428   | 13  | 7   | 20.767      | 30          | 1314  |
| 8   | 2   | 11.196      | 10          | 438   |     |     |             |             | 0.464 |
| 8   | 0   | 11.434      | 2           | 440   | 15  | 13  | 21.231      | 54          | 1368  |
Table 2: Magic numbers provided by the 3-dimensional $q$-deformed harmonic oscillator (Table 1), reported in column 1, are compared to the experimental data of Martin et al. [111] (column 2), Bjørnholm et al. [112] (column 3), Knight et al. [113] (column 4), Pedersen et al. [115] (column 5) and Bréchignac et al. [116] (column 6), concerning Na clusters. The magic numbers provided [118] by the (non-deformed) 3-dimensional harmonic oscillator (column 9), the square well potential (column 8) and a rounded square well potential intermediate between the previous two (column 7) are also shown for comparison. See text for discussion.

| present | exp. [111] | exp. [112] | exp. [113] | exp. [115] | exp. [116] | int. [118] | sq. well [118] | h. osc. [118] |
|---------|-----------|-----------|-----------|-----------|-----------|-----------|---------------|-------------|
| 2       | 2         | 2         | 2         | 2         | 2         | 2         | 2             | 2           |
| 8       | 8         | 8         | 8         | 8         | 8         | 8         | 8             | 8           |
| (18)    | 18        |           |           |           |           |           | 18            | 18          |
| 20      | 20        | 20        | 20        | 20        | 20        | 20        | 20            | 20          |
| 34      | 34        |           |           |           |           |           | 34            | 34          |
| 40      | 40        | 40        | 40        | 40        | 40        | 40        | 40            | 40          |
| 58      | 58        | 58        | 58        | 58        | 58        | 58        | 68,70         | 68          |
| 92      | 90,92     | 92        | 92        | 92        | 92        | 92        | 90,92         | 92          |
| 92      | 106,112   | 106       | 112       |           |           |           |               |             |
| 138     | 138       | 138       | 138       | 134       | 138       | 132,138    |               |             |
| 198     | 198±2     | 196       | 198       | 191       | 156       | 156       | 168           |             |
| 254     | 260±4     |           |           |           |           |           |               |             |
| 268     | 263±5     | 264       | 262       |           |           |           |               |             |
| 338     | 341±5     | 344±4     | 344       | 342       |           |           |               |             |
| 440     | 443±5     | 440±2     | 442       | 442       |           |           |               |             |
| 556     | 557±5     | 558±8     | 554       | 552       |           |           |               |             |
| 676     |           |           |           |           |           |           | 680           |             |
| 694     | 700±15    |           |           |           |           |           | 695           |             |
| 832     | 840±15    | 800       | 822       |           |           |           |               |             |
| 912     |           |           |           |           |           |           | 902           |             |
| 1012    | 1040±20   | 970       | 1025      |           |           |           |               |             |
| 1100    |           |           |           |           |           |           | 1120          |             |
| 1206    | 1220±20   |           |           |           |           |           |               |             |
| 1284    |           |           |           |           |           |           | 1297          |             |
| 1314    |           |           |           |           |           |           | 1310          |             |
| 1410    | 1430±20   |           |           |           |           |           |               |             |
| 1502    |           |           |           |           |           |           | 1500          |             |
Table 3: Magic numbers provided by the 3-dimensional $q$-deformed harmonic oscillator (Table 1), reported in column 1, are compared to the experimental data of Martin et al. [111] (column 2), Pedersen et al. [115] (column 3), and Bréchignac et al. [116] (column 4), as well as to the theoretical predictions of various jellium model calculations reported by Martin et al. [111] (column 5), Bjørnholm et al. [112] (column 6), Brack [73] (column 7), Bulgac and Lewenkopf [74] (column 8), the theoretical predictions of Woods–Saxon and wine bottle potentials reported by Nishioka et al. [125] (column 9), as well as to the magic numbers predicted by the classification scheme using the $3n + l$ pseudo quantum number, reported by Martin et al. [111] (column 10). See text for discussion.

| Present | Exp. [111] | Exp. [115] | Exp. [116] | Jell. [111] | Jell. [112] | Jell. [73] | Jell. [74] | WS | 3n + l |
|---------|------------|------------|------------|------------|------------|------------|------------|----|--------|
| 2       | 2          | 2          | 2          | 2          | 2          | 2          | 2          |    |        |
| 8       | 8          | 8          | 8          | 8          | 8          | 8          | 8          |    |        |
| (18)    | 18         | 18         | 18         | 18         | 18         | 18         | 18         |    |        |
| 20      | 20         | (20)       | 20         | 20         | 20         | 18         | 20         |    |        |
| 34      | 34         | 34         | 34         | 34         | 34         | 34         | 34         |    |        |
| 40      | 40         | 40         | (40)       | 40         | 40         | 40         | 40         |    |        |
| 58      | 58         | 58         | 58         | 58         | 58         | 58         | 58         |    | 68     |
| 92      | 90,92      | 92         | 93         | 92         | 92         | 92         | 92         |    | 90     |
| 138     | 138        | 138        | 134        | 134        | 138        | 138        | 138        |    | 132    |
| 198     | 198±2      | 198        | 191        | (196)      | 196        | 196        | 198        |    |        |
| 254     |            |            | 254        | 254        | 254        | 254        | 254        |    |        |
| 268     | 263±5      | 264        | 262        | (268)      |            |            |            |    |        |
| 338     | 341±5      | 344        | 342        | 338(356)   | 338        | 338        | 338        |    | 332    |
| 440     | 443±5      | 442        | 442        | 440        | 440        | 440        | 440        |    | 428    |
| 556     | 557±5      | 554        | 552        | 562        | 556        | 556        | 556        |    | 562    |
| 676     | 680        |            | 676        | 676        | 676        | 676        | 676        |    |        |
| 694     | 700±15     | 695        | 704        |            |            |            |            |    | 694    |
| 832     | 840±15     | 800        | 822        | 852        | 832        | 832        | 832        |    | 820    |
| 912     |            | 902        |            | 912        |            | 912        |            |    |        |
| 1012    | 1040±20    | 970        | 1025       | 1074       | 1074       | 1012       | 990        |    |        |
| 1100    |            |            | 1120       | 1100       | 1100       | 1100       | 1100       |    |        |
| 1206    | 1220±20    |            |            |            |            |            |            | 1216| 1182   |
| 1284    |            |            | 1297       |            |            |            |            | 1284| 1284   |
| 1314    |            |            |            |            |            |            |            | 1314|        |
| 1410    | 1430±20    |            |            |            |            |            |            |    | 1398   |
| 1502    | 1500       |            |            |            |            |            |            | 1502| 1516   |