QUANTUM ALGEBRAIC SYMMETRIES IN ATOMIC CLUSTERS, MOLECULES AND NUCLEI

Dennis Bonatsos and N. Karoussos
Institute of Nuclear Physics, NCSR “Demokritos”
GR-15310 Aghia Paraskevi, Attiki, Greece

P. P. Raychev and R. P. Roussev
Institute for Nuclear Research and Nuclear Energy
72 Tzarigrad Road, BG-1784 Sofia, Bulgaria

1. INTRODUCTION

Quantum algebras (also called quantum groups) 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 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. 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, hydrogen atom and hydrogen-like spectra, rotational and vibrational nuclear and molecular spectra, and in conformal field theories. By now much work has been done on the $q$-deformed oscillator and its relativistic extensions, and several kinds of generalized deformed oscillators and $su(2)$ algebras have been introduced. Simple and self-contained introductions to the quantum algebraic techniques and their applications in physics can be found in Refs [1–3].

Here we shall confine ourselves to a list of applications of quantum algebras in nuclear structure physics and in molecular physics and, in addition, a recent application of quantum algebraic techniques to the structure of atomic clusters will be discussed in more detail.

2. QUANTUM ALGEBRAS IN NUCLEAR STRUCTURE

We give here a brief list of applications of quantum algebraic techniques in nuclear structure. More details and relevant references can be found in the review
1) Rotational spectra of deformed and superdeformed nuclei, including excited (beta and gamma) bands, have been described in terms of the $su_q(2)$ model, in a way similar to that provided by the Variable Moment of Inertia (VMI) model, with the deformation parameter $\tau$ (with $q = e^{i\tau}$) found 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 and to the nuclear deformation $\beta$. Recently the model has been extended in order to be applicable to transitional and vibrational spectra.

2) $B(E2)$ transition probabilities have also been described in the framework of the $su_q(2)$ model. 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.) 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, along with theoretical predictions from other models towards the same direction.

3) A generalization of the $su_q(2)$ model is based on the use of the deformed algebra $su_\Phi(2)$, 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 $\Phi$. 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.

4) It has been found that correlated fermion pairs coupled to zero angular momentum in a single-$j$ shell behave approximately as suitably defined $q$-deformed bosons, the pairing energies also being correctly reproduced up to the same order, and the deformation parameter ($\tau = \ln q$) being found to be inversely proportional to the size of the shell. The same system of correlated fermion pairs can be described exactly by suitably defined generalized deformed bosons. 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.

5) A $q$-deformed version of a two dimensional toy Interacting Boson Model (IBM) with $su_q(3)$ overall symmetry, as well as $q$-deformed versions of the $o(6)$ and $u(5)$ limits of the full IBM have been developed. The $q$-deformation of the $su(3)$ limit of IBM is a formidable problem, since the $su_q(3)$ $\supset so_q(3)$ decomposition has for the moment been achieved only for completely symmetric $su_q(3)$ irreducible representations.

6) A $q$-deformed version of the Moszkowski model as well as a $q$-deformed Moszkowski model with cranking have been developed. The possibility of using $q$-deformation in assimilating temperature effects is receiving attention, since it has also been found 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 $su_q(2)$ algebra, and for the 3-level version of the model in terms of an $su_q(3)$ algebra.

7) It has been proved that a generalized deformed $u(2)$ algebra is the symmetry algebra of the two-dimensional anisotropic quantum harmonic oscillator with rational ratios of frequencies (RHO), which is the oscillator describing the single-particle level.
spectrum of “pancake” nuclei, i.e. of very oblate triaxially deformed nuclei with \( \omega_x \gg \omega_y, \omega_z \). Furthermore, a generalized deformed \( u(3) \) algebra turns out to be the symmetry algebra of the three-dimensional RHO, which is related to the symmetry underlying the structure of superdeformed and hyperdeformed nuclei.

8) Recently the 3-dimensional \( q \)-deformed (isotropic) harmonic oscillator has been studied in detail [4]. 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. An appropriate \( q \)-deformed spin–orbit interaction term has also been developed [4]. 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.

3. 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. More details and relevant references can be found in the review articles [1–3].

1) Rotational spectra of diatomic molecules have been described in terms of the \( su_q(2) \) model. 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. Molecular backbending (bandcrossing) has also been described in this framework. Rotational spectra of symmetric top molecules have also been considered in the framework of the \( su_q(2) \) symmetry. Furthermore, two \( q \)-deformed rotors with slightly different parameter values have been used for the description of \( \Delta I = 1 \) staggering effects in rotational bands of diatomic molecules.

2) Vibrational spectra of diatomic molecules have been described in terms of \( q \)-deformed anharmonic oscillators having the \( su_q(1,1) \) or the \( u_q(2) \supset o_q(2) \) symmetry, as well as in terms of generalized deformed oscillators. These results, combined with 1), lead to the full summation of the Dunham expansion. A two-parameter deformed anharmonic oscillator with \( u_{qp}(2) \supset o_{qp}(2) \) symmetry has also been considered.

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 providing approximately the same spectrum. The results have been corroborated by the study of the relation between \( su_q(1,1) \) and the anharmonic oscillator with \( x^4 \) anharmonicities. Furthermore the WKB-EP corresponding to the \( su_q(1,1) \) anharmonic oscillator has been connected to a class of Quasi-Exactly Soluble Potentials (QESPs).

4) Generalized deformed oscillators giving the same spectrum as the Morse potential and the modified Pöschl–Teller potential, as well as a deformed oscillator containing them as special cases have also been constructed. In addition, \( q \)-deformed versions of the Morse potential have been given, either by using the \( so_{q}(2,1) \) symmetry or by solving a \( q \)-deformed Schrödinger equation for the usual Morse potential. 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.
5) A $q$-deformed version of the vibron model for diatomic molecules has been constructed.

6) For vibrational spectra of polyatomic molecules a model of $n$ coupled generalized deformed oscillators has been built, containing the approach of Iachello and Oss as a special case. In addition a model of two $Q$-deformed oscillators coupled so that the total Hamiltonian has the $su_Q(2)$ symmetry has been proved 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.

4. QUANTUM ALGEBRAIC SYMMETRIES IN ATOMIC CLUSTERS

4.1 Introduction

In this Section we will discuss in some detail an application of quantum algebraic techniques to atomic clusters. Because of lack of space, no detailed list of references will be given. For the relevant references the reader is referred to Refs [4–6].

Metal clusters have been recently the subject of many investigations. One of the first fascinating findings in their study was the appearance of magic numbers, analogous to but different from the magic numbers appearing in the shell structure of atomic nuclei. Different kinds of metallic clusters [alkali metals (Na, Li, K, Rb, Cs), noble metals (Cu, Ag, Au), divalent metals of the IIB group (Zn, Cd), trivalent metals of the III group (Al, In)] exhibit different sets of magic numbers. The analogy between the magic numbers observed in metal clusters and the magic numbers observed in atomic nuclei led to the early description of metal clusters in terms of the Nilsson–Clemenger model, which is a simplified version of the Nilsson model of atomic nuclei, in which no spin-orbit interaction is included. Further theoretical investigations in terms of the jellium model 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. 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. Again in this case the intermediate potential resembles a harmonic oscillator flattened at the bottom.

On the other hand, modified versions of harmonic oscillators have been recently investigated in the novel mathematical framework of quantum algebras, which are nonlinear generalizations of the usual Lie algebras. 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, while the corresponding (WKB-equivalent) potentials 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 [4], taking advantage of the \( u_q(3) \supset \text{so}_q(3) \) symmetry. The spectrum of this 3-dimensional \( q \)-deformed harmonic oscillator has been found [4] to reproduce very well the spectrum of the modified harmonic oscillator introduced by Nilsson, 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, 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.

4.2 The 3-dimensional \( q \)-deformed harmonic oscillator

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, \( \text{so}_q(3) \), can be defined [4]. The Hamiltonian of the 3-dimensional \( q \)-deformed harmonic oscillator is defined so that it satisfies the following requirements:

a) It is an \( \text{so}_q(3) \) scalar, i.e. the energy is simultaneously measurable with the \( q \)-deformed angular momentum related to the algebra \( \text{so}_q(3) \) and its \( z \)-projection.

b) It conserves the number of bosons, in terms of which the quantum algebras \( u_q(3) \) and \( \text{so}_q(3) \) 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 [4] 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 \( \text{so}_q(3) \), 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 [4]

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

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 [4]

$$E_q(n, l) = \hbar \omega_0 n - \hbar \omega_0 \tau (l(l + 1) - n(n + 1))$$

$$- \hbar \omega_0 \tau^2 \left( l(l + 1) - \frac{1}{3} n(n + 1)(2n + 1) \right) + O(\tau^3). \quad (4)$$

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

$$V = \frac{1}{2} \hbar \omega \rho^2 - \hbar \omega \mu' (L^2 - <L^2>_N), \quad \rho = r \sqrt{\frac{M \omega}{\hbar}}, \quad <L^2>_N = \frac{N(N + 3)}{2}. \quad (5)$$

The energy eigenvalues of Nilsson’s modified harmonic oscillator are

$$E_{nl} = \hbar \omega n - \hbar \omega \mu' \left( l(l + 1) - \frac{1}{2} n(n + 3) \right). \quad (6)$$

It has been proved [4] 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.

In the spectrum of the 3-dimensional $q$-deformed harmonic oscillator each level is characterized by the quantum numbers $n$ (number of vibrational quanta) and $l$ (angular momentum). The number of particles which can be accommodated by a level with angular momentum $l$ is equal to $2(2l + 1))$. The total number of particles up to and including this level is given by the sum of the quantity $2(2l + 1)$ for all levels up to and including the level in question. If the energy difference between two successive levels is larger than a given number, which for future reference we call $\delta$, it is considered as a gap separating two successive shells, so that the number of particles which can be accommodated up to the gap is a magic number. If the energy separation is smaller than $\delta$, the successive levels are considered as belonging to the same shell and no magic number occurs at this point.

In Table 1 of Ref. [5] and in Tables 1, 2, 3 of Ref. [6] one can find various level schemes of the 3-dimensional $q$-deformed harmonic oscillator for various values of the deformation parameter ($\tau = 0.020, 0.038, 0.050$) and the energy gap ($\delta = 0.20, 0.26, 0.38, 0.39$). We remark that the small magic numbers do not change much as the parameter $\tau$ is varied, while large magic numbers get more influenced by the parameter modification.

### 4.3 Sodium and lithium clusters

The magic numbers provided by the 3-dimensional $q$-deformed harmonic oscillator with $\tau = 0.038$ and $\delta = 0.39$ have been compared to available experimental data for Na clusters and Li clusters in Table 4 of Ref. [6]. 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. 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.

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 results of the four experiments, which report magic numbers in this region, are quite different. However, the results of all four experiments are well accommodated by the present model. In addition, each magic number predicted by the model is supported by at least one experiment.

In Table 4 of Ref. [6] the predictions of three simple theoretical models (non-deformed 3-dimensional harmonic oscillator, square well potential, rounded square well potential (intermediate between the previous two)) 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, this assumption being applicable under conditions not favoring delocalization of the valence electrons of alkali atoms.

Comparisons among the present results, experimental data for Na and Li clusters, and theoretical predictions more sophisticated than these reported in Table 4 of Ref. [6], have been made in Table 5 of Ref. [6], where magic numbers predicted by various jellium model calculations, Woods–Saxon and wine bottle potentials, as well as by a classification scheme using the $3n + l$ pseudo quantum number 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. Woods–Saxon and wine bottle potentials 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 of Ref. [6]), 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.
Experimental data for various alkali metal clusters (Li, Na, K, Rb, Cs) and noble metal clusters (Cu, Ag, Au) have been reported in Table 6 of Ref. [6], along with the theoretical predictions of the 3-dimensional $q$-deformed harmonic oscillator with $\tau = 0.038$ and $\delta = 0.39$. The following comments apply:

i) In the cases of Rb, Cu, Ag, and Au, what is seen experimentally is cations of the type $\text{Rb}^+_N$, $\text{Cu}^+_N$, $\text{Ag}^+_N$, $\text{Au}^+_N$, which contain $N$ atoms each, but $N - 1$ electrons. The magic numbers reported in Table 6 of Ref. [6] are electron magic numbers in all cases.

ii) All alkali metals and noble metals give the same magic numbers, at least within the ranges reported in the table. For most of these metals the range of experimentally determined magic numbers is rather limited, with Na, Cs, Li, and Ag being notable exceptions.

iii) The magic numbers occurring in Na, Cs, Li, and Ag are almost identical, and are described very well by the 3-dimensional $q$-deformed harmonic oscillator with $\tau = 0.038$ and $\delta = 0.39$. The limited data on K, Rb, Cu, Au, also agree with the magic numbers of the same oscillator.

### 4.5 Divalent metals of the IIB group

For these metals the quantities determined experimentally are numbers of atoms exhibiting “magic” behaviour. Each atom has two valence electrons, therefore the magic numbers of electrons are twice the magic numbers of atoms. The magic numbers of electrons for Zn and Cd clusters have been reported in Table 7 of Ref. [6], along with the magic numbers predicted by the 3-dimensional $q$-deformed harmonic oscillator for two different parameter values ($\tau = 0.038$, $\delta = 0.26$ and $\tau = 0.020$, $\delta = 0.20$), and the magic numbers given by a potential intermediate between the simple harmonic oscillator and the square well potential. The following comments can be made:

i) The experimental magic numbers for Zn and Cd are almost identical. Magic numbers reported in parentheses are “secondary” magic numbers, while the magic numbers without parentheses are the “main” ones, as indicated in the experimental papers.

ii) In Table 7 of Ref. [6] magic numbers of the 3-dimensional $q$-deformed harmonic oscillator with $\tau = 0.038$ and energy gaps larger than 0.26 are reported. Decreasing the energy gap considered as separating different shells from 0.39 (used in Table 1 of Ref. [6]) to 0.26 (used in Table 7 of Ref. [6]) has as a result that the numbers 70 and 106 become magic, in close agreement with the experimental data. Similar but even better results are gotten from the 3-dimensional $q$-deformed harmonic oscillator characterized by $\tau = 0.020$, with the energy gap between different shells being set equal to 0.20. We observe that the second oscillator predicts an additional magic number at 112, in agreement with experiment, but otherwise gives the same results as the first one. We remark therefore that the general agreement between the results given by the 3-dimensional $q$-deformed harmonic oscillator and the experimental data
is not sensitively dependent on the parameter value, but, in contrast, quite different parameter values ($\tau = 0.038$, $\tau = 0.020$) provide quite similar sets of magic numbers (at least in the region of relatively small magic numbers).

iii) Both oscillators reproduce all the “main” magic numbers of Zn and Cd, while the intermediate potential between the simple harmonic oscillator and the square well potential, reported in the same table, reproduces all the “main” magic numbers except 106.

4.6 Trivalent metals of the III group

Magic numbers of electrons for the trivalent metals Al and In are reported in Table 7 of Ref. [6], along with the predictions of the 3-dimensional $q$-deformed harmonic oscillator with $\tau = 0.050$ and $\delta = 0.38$. The following comments can be made:

i) It is known that small magic numbers in clusters of Al and In cannot be explained by models based on the filling of electronic shells, because of symmetry breaking caused by the ionic lattice, while for large magic numbers this problem does not exist.

ii) The 3-dimensional $q$-deformed harmonic oscillator with $\tau = 0.050$ and $\delta = 0.38$ provides magic numbers which agree quite well with the experimental findings, with an exception in the region of small magic numbers, where the model fails to reproduce the magic numbers 164 and 198, predicting only a magic number at 186. In addition the oscillator predicts magic numbers at 398, 890, 1074, which are not seen in the experiment.

4.7 Discussion

The following general remarks can now be made:

i) From the results reported above it is quite clear that the 3-dimensional $q$-deformed harmonic oscillator describes very well the magic numbers of alkali metal clusters and noble metal clusters in all regions, using only one free parameter ($q = e^{\tau}$ with $\tau = 0.038$). It also provides an accurate description of the “main” magic numbers of clusters of divalent group IIB metals, either with the same parameter value ($\tau = 0.038$) or with a different one ($\tau = 0.020$). In addition it gives a satisfactory description of the magic numbers of clusters of trivalent group III metals with a different parameter value ($\tau = 0.050$).

ii) It is quite remarkable that the 3-dimensional $q$-deformed harmonic oscillator reproduces long sequences of magic numbers (Na, Cs, Li, Ag) at least as accurately as other, more sophisticated, models by using only one free parameter ($q = e^{\tau}$). 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.

iii) It has been remarked 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 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 $u(3)$.

iv) 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 Refs [1,2]. The similarity between the results of the present model and these provided by the Woods–Saxon potential (Table 5 of Ref. [6]) 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, remains to be seen.

In summary, we have shown 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 and of noble metal clusters up to 1500, which is the expected limit of validity for theories based on the filling of electronic shells. In addition it gives a good description of the “main” magic numbers of group IIB (divalent) metal clusters, as well as a satisfactory description of group III (trivalent) metal clusters. 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 several metal clusters.

REFERENCES