Unified description of magic numbers of metal clusters in terms of the 3-dimensional $q$-deformed harmonic oscillator

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Abstract

Magic numbers predicted by a 3-dimensional $q$-deformed harmonic oscillator with $u_q(3)$ ⊃ so$_q$(3) symmetry are compared to experimental data for atomic clusters of alkali metals (Li, Na, K, Rb, Cs), noble metals (Cu, Ag, Au), divalent metals (Zn, Cd), and trivalent metals (Al, In), as well as to theoretical predictions of jellium models, Woods–Saxon and wine bottle potentials, and to the classification scheme using the $3n + l$ pseudo quantum number. In alkali metal clusters and noble metal clusters the 3-dimensional $q$-deformed harmonic oscillator correctly predicts all experimentally observed magic numbers up to 1500 (which is the expected limit of validity for theories based on the filling of electronic shells), while in addition it gives satisfactory results for the magic numbers of clusters of divalent metals and trivalent metals, thus indicating that $u_q(3)$, which is a nonlinear extension 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. The Taylor expansions of angular momentum dependent potentials approximately producing the same spectrum as the 3-dimensional $q$-deformed harmonic oscillator are found to be similar to the Taylor expansions of the symmetrized Woods–Saxon and “wine-bottle” symmetrized Woods–Saxon potentials, which are known to provide successful fits of the Ekardt potentials.

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1. Introduction

Metal clusters have been recently the subject of many investigations (see [1, 2, 3, 4] for relevant reviews). 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 [5]. Different kinds of metallic clusters [alkali metals (Na [6, 7, 8, 9], Li [10, 11], K [12], Rb [13], Cs [7, 14, 15]), noble metals (Cu [16, 17], Ag [10, 18], Au [16]), divalent metals of the IIB group (Zn, Cd) [19], trivalent metals of the III group (Al, In) [20]) 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 [21], which is a simplified version of the Nilsson model [22, 23] of atomic nuclei, in which no spin-orbit interaction is included. Further theoretical investigations in terms of the jellium model [24, 25] 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 [24, 27]. 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 [1]. Again in this case the intermediate potential resembles a harmonic oscillator flattened at the bottom.

On the other hand, modified versions of harmonic oscillators [28, 29] have been recently investigated in the novel mathematical framework of quantum algebras [30, 31], 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 [22], while the corresponding (equivalent within the limits of perturbation theory or WKB-equivalent) potentials [33, 34] 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 [35], taking advantage of the $u_q(3) \supset so_q(3)$ symmetry [30, 37]. The spectrum of this 3-dimensional $q$-deformed harmonic oscillator has been found [35] to reproduce very well the spectrum of the modified harmonic oscillator introduced by Nilsson [22, 23] 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 [21], it is worth examining if the 3-dimensional $q$-deformed harmonic oscillator can reproduce the magic numbers of simple metallic clusters and, in the case that this is possible, to determine potentials giving the same spectrum as this oscillator and compare them to the symmetrized Woods–Saxon and “wine-bottle” symmetrized Woods–Saxon potentials, which successfully fit [26, 27] the Ekardt potentials [24]. These are the subjects of the present investigation.

It is worth mentioning at this point that an effort has been made to describe the magic numbers of metal clusters by a quantum number $3n + l$ [6], where $n$ is the number of nodes in the solution of the radial Schrödinger equation and $l$ is the angular momentum quantum number. This approach has been inspired by the fact that degenerate energy levels in the hydrogen atom are characterized by the same value of the quantum number $n + l$, due to
the so(4) symmetry underlying this system, while degenerate energy levels in the spherical harmonic oscillator (i.e. the 3-dimensional isotropic harmonic oscillator) are characterized by the same value of the parameter $2n + l$, due to the su(3) symmetry underlying this system. The $3n + l$ quantum number has been used [6] to approximate the magic numbers of alkali metal clusters with some success, and focusing potentials characterized by this degeneracy have been determined [38], but no relevant Lie symmetry could be determined [38, 39].

In Section 2 the 3-dimensional $q$-deformed harmonic oscillator will be briefly described, while in Section 3 the magic numbers provided by this oscillator will be compared with the experimental data for Na and Li clusters, as well as with the predictions of other theories (jellium model, Woods–Saxon and “wine bottle” potentials, classification scheme using the $3n + l$ pseudo quantum number). Additional comparisons of magic numbers predicted by the 3-dimensional $q$-deformed harmonic oscillator to experimental data and to the results of other theoretical approaches will be made in Section 4 (for other alkali metal clusters and noble metal clusters), Section 5 (for divalent group IIB metal clusters), and Section 6 (for trivalent group III metal clusters), while in Section 7 potentials giving approximately the same spectrum as the 3-dimensional $q$-deformed harmonic oscillator will be determined and subsequently compared to the symmetrized Woods–Saxon and “wine-bottle” symmetrized Woods–Saxon potentials. Finally, Section 8 will contain discussion of the present results and plans for further work.

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, $so_q(3)$, can be defined [35]. 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 $q \rightarrow 1$ it is in agreement with the Hamiltonian of the usual 3-dimensional harmonic oscillator.

It has been proved [35] 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 [35]

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

\[
E_q(n, l) = \hbar \omega_0 n - \hbar \omega_0 \tau (l(l+1) - n(n+1)) - \hbar \omega_0 \tau^2 \left( l(l+1) - \frac{1}{3} n(n+1)(2n+1) \right) + O(\tau^3). \tag{4}
\]

The last expression to leading order bears great similarity to the modified harmonic oscillator suggested by Nilsson \[22, 23\] (with the spin-orbit term omitted)

\[
V = \frac{1}{2} \hbar \omega \rho^2 - \hbar \omega \kappa' (L^2 - < L^2 >_N), \quad \rho = r \sqrt{\frac{M \omega}{\hbar}}, \tag{5}
\]

where

\[
<L^2 >_N = \frac{N(N+3)}{2}. \tag{6}
\]

The energy eigenvalues of Nilsson’s modified harmonic oscillator are \[22, 23\]

\[
E_{nl} = \hbar \omega n - \hbar \omega \mu' \left( l(l+1) - \frac{1}{2} n(n+3) \right). \tag{7}
\]

It has been proved \[23\] 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, 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, which we shall denote by \( \delta \), 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.

Additional level schemes of the 3-dimensional \( q \)-deformed harmonic oscillator are given in Table 2 (for \( \tau = 0.020 \) and energy gap \( \delta = 0.20 \)) and in Table 3 (for \( \tau = 0.050 \) and energy gap \( \delta = 0.38 \)). The following remarks are now in place:

i) Small magic numbers do not change much as the parameter \( \tau \) is varied (taking positive values), while large magic numbers get more influenced by the parameter modification. In general, the ordering of the levels does not change rapidly with the value of the parameter \( \tau \) (for \( \tau > 0 \)).

ii) Rapid change of the magic numbers as a function of \( \tau \) occurs when \( \tau \) takes negative values, but this case is irrelevant to the contents of the present work.
iii) Magic numbers are influenced more drastically by the value of the energy gap $\delta$. If in the spectrum obtained for a given value of the parameter $\tau$ the energy separation between two successive levels is only slightly smaller than the energy gap $\delta$, this can be considered as an indication of the presence of a “secondary” magic number. (See the end of Section 3 for specific examples.)

3. Sodium and lithium clusters

The magic numbers provided by the 3-dimensional $q$-deformed harmonic oscillator in Table 1 are compared to available experimental data for Na clusters [6, 7, 8, 9] and Li clusters [10, 11] in Table 4 (columns 2–7). Some preliminary results concerning Na clusters have already been given earlier in Ref. [12]. 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 [6]. 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 [13].

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 the predictions of three simple theoretical models [14] (non-deformed 3-dimensional harmonic oscillator (column 10), square well potential (column 9), rounded square well potential (intermediate between the previous two, column 8) ) 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 [15], 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 clusters (by Martin et al. [6] (column 2) and Pedersen et al. [9] (column 3)), experimental data for Li clusters (Bréchignac et al. [10] (column 4) ), and theoretical predictions more sophisticated than these reported in Table 4, can be made in Table 5, where magic numbers predicted by various jellium model calculations (columns 5–8, [16, 17, 18, 19, 20, 21]), Woods–Saxon and wine bottle potentials (column 9, [22]), as well as by a classification scheme using the $3n + l$ pseudo quantum number (column 10, [3]) 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. [13] 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.

4. Other alkali metals and noble metals

Experimental data for various alkali metal clusters [Li ([10], column 2), Na ([6], column 3), K ([12], column 4), Rb ([13], column 5), Cs ([7, 14], column 6)] and noble metal clusters [Cu ([16], column 7), Ag ([15], column 8 and [16] in column 9), Au ([16], column 10)] are reported in Table 6, along with the theoretical predictions of the 3-dimensional $q$-deformed harmonic oscillator given in Table 1. The following comments apply:

i) In the cases of Rb [13], Cu [16], Ag [16], Au [16], what is seen experimentally is cations of the type $Rb^+_N$, $Cu^+_N$, $Ag^+_N$, $Au^+_N$, which contain $N$ atoms each, but $N − 1$ electrons. The magic numbers reported in Table 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 [6], Cs [7, 14], Li [10], and Ag [18] being notable exceptions.

iii) The magic numbers occurring in Na [6], Cs [7, 14], Li [10], and Ag [18] are almost identical, and are described very well by the 3-dimensional $q$-deformed harmonic oscillator of Table 1. The limited data on K, Rb, Cu, Au, also agree with the magic numbers of Table 1.

5. Divalent metals of the IIB group

For these metals the quantities determined experimentally [19] 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 [13] are reported in Table 7 (in columns 4 and 5 respectively), along with the magic numbers predicted by the 3-dimensional $q$-deformed harmonic oscillator for two different parameter values (given in Tables 1 and 2 and reported in columns 1 and 2 respectively), and the magic numbers given by a potential intermediate between the simple harmonic oscillator and the square well potential ([19], column 3). The following comments can be made:

i) The experimental magic numbers for Zn and Cd [14] 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 [1].

ii) In column 1 of Table 7 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 $\delta$ considered as separating different shells from 0.39 (used in Table 1) to 0.26 (used in Table 7) 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 of Table 2, reported in column 2 of Table 7. This oscillator is characterized by $\tau = 0.020$, while the energy gap $\delta$ between different shells is 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 column 3, reproduces all the “main” magic numbers except 108.

6. Trivalent metals of the III group

Magic numbers of electrons for the trivalent metals Al and In [20] are reported in Table 7 (in columns 7 and 8 respectively), along with the predictions of the 3-dimensional $q$-deformed harmonic oscillator of Table 3 (column 6). The following comments can be made:

i) It is known [1, 20] 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 [20], while for large magic numbers this problem does not exist.

ii) The 3-dimensional $q$-deformed harmonic oscillator of Table 3 provides the magic numbers reported in column 6 of Table 7. These magic numbers 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 reported in column 7.

7. Potentials corresponding to the 3-dimensional $q$-deformed harmonic oscillator

As we have seen in the previous sections, the 3-dimensional $q$-deformed harmonic oscillator describes successfully the magic numbers of several metallic clusters. On the other hand, it is known that metallic clusters are successfully described by the Ekardt potentials [24] (for which analytical expressions are lacking), which have been recently parametrized in terms of symmetrized Woods–Saxon and “wine-bottle” symmetrized Woods–Saxon potentials [26, 27] (for which analytical expressions are known). Therefore the following questions are created:

a) Is it possible to determine some potentials which, when put into the Schrödinger equation, will provide approximately the same spectrum as the 3-dimensional $q$-deformed harmonic oscillator?

b) If such potentials can be found, how do they compare with the symmetrized Woods–Saxon and “wine-bottle” symmetrized Woods–Saxon potentials?

Question a) is a standard problem of inverse scattering [44]. Classical potentials giving approximately the same spectrum as the one-dimensional $q$-deformed harmonic oscillator have been determined either through use of standard perturbation theory [33], or within the limits of the WKB approximation [34].

In what follows we are going to determine potentials giving approximately the same spectrum as the 3-dimensional $q$-deformed harmonic oscillator by using the method of Ref. [33], i.e. perturbation theory. According to this method, a potential of the form

$$V = V_0 + \kappa x^2 + \lambda x^4 + \mu x^6 + \xi x^8 + \cdots$$

(8)
corresponds, in first-order perturbation theory and keeping terms up to $x^8$ only, to a spectrum

$$E = \varepsilon_0 + \kappa + 3\lambda + 15\mu + 105\xi + (2\kappa + 6\lambda + 40\mu + 280\xi)n$$

7
potential.

In order to do this, for each possible value of \(l\) (\(l = n, n - 2, n - 4, \ldots 1\) or 0) can be put in the form:

\[
\lambda = \text{order to do this, for each possible value of } l (l = n, n - 2, n - 4, \ldots 1 \text{ or } 0) \text{ can be put in the form:}
\]

\[
E_q(n, n) = \hbar \omega_0 [n]_q^2 \quad \text{for} \quad l = n, \quad (10)
\]

\[
E_q(n, n - 2) = \hbar \omega_0 (q^2[n - 1]_q^2 + q^{2n}) \quad \text{for} \quad l = n - 2, \quad (11)
\]

\[
E_q(n, n - 4) = \hbar \omega_0 (q^4[n - 2]_q^2 + q^{2(n-1)}[2]_q^2) \quad \text{for} \quad l = n - 4, \quad (12)
\]

\[
E_q(n, n - 6) = \hbar \omega_0 (q^6[n - 3]_q^2 + q^{2(n-2)}[3]_q^2) \quad \text{for} \quad l = n - 6, \quad (13)
\]

\[
E_q(n, 3) = \hbar \omega_0 (q^8[n - 3]_q^2 + q^{-4}[5]_q^2 - q^{-2}[3]_q^2 + 1)
\]

\[
= E_q(n, 0) - \hbar \omega_0 (q^6 - 1)(1 + q^{-4}) \quad \text{for} \quad l = 3, \quad (14)
\]

\[
E_q(n, 2) = \hbar \omega_0 (q^4[n - 2]_q^2 + q^{-2}[3]_q^2 - 1) = E_q(n, 0) - \hbar \omega_0 (q^4 - q^{-2}) \quad \text{for} \quad l = 2, \quad (15)
\]

\[
E_q(n, 1) = \hbar \omega_0 (q^4[n - 1]_q^2 + 1) = E_q(n, 0) - \hbar \omega_0 (q^2 - 1) \quad \text{for} \quad l = 1, \quad (16)
\]

\[
E_q(n, 0) = \hbar \omega_0 q^2[n]_q \quad \text{for} \quad l = 0, \quad (17)
\]

where by \([n]_q\) are denoted the \(q\)-numbers of Eq. (2), which are symmetric under the exchange \(q \leftrightarrow q^{-1}\), while by \([[n]]_q\) are denoted the \(q\)-numbers

\[
[[n]]_q = \frac{q^n - 1}{q - 1}, \quad (18)
\]

which are not symmetric under the exchange \(q \leftrightarrow q^{-1}\). For all of these equations it is clear that they reduce to the classical expression \(E(n) = \hbar \omega_0 n\) in the limit \(q \to 1\).

We then consider the Taylor expansions for these energy expressions. By comparing them to Eq. (9) and equating the coefficients of the various powers of \(n\) (up to \(n^4\)) we determine in each case the coefficients \(\kappa, \lambda, \mu, \xi\). Substituting these coefficients in Eq.
(8) we determine for each case the corresponding potential, keeping terms up to $\tau^4$ (where $q = e^\tau$). The first few cases are:

\[
\frac{V(x)}{\hbar \omega_0} = -\left(\frac{1}{2} - \frac{\tau^2}{2} + \frac{4\tau^4}{15}\right) + \left(\frac{1}{2} - \frac{\tau^2}{2} + \frac{4\tau^4}{15}\right) x^2
\]

\[
- \left(\frac{\tau^2}{6} - \frac{\tau^4}{9}\right) x^4 + \left(\frac{\tau^2}{30} - \frac{\tau^4}{45}\right) x^6 \quad \text{for } l = n,
\]

\[
\frac{V(x)}{\hbar \omega_0} = -\left(\frac{1}{2} + 4\tau + \frac{7\tau^2}{2} + \frac{8\tau^3}{3} + \frac{8\tau^4}{5}\right) + \left(\frac{1}{2} + 2\tau + \frac{3\tau^2}{2} + \frac{10\tau^3}{3} + \frac{44\tau^4}{15}\right) x^2
\]

\[
- \left(\frac{\tau^2}{6} + \frac{4\tau^3}{3} + \frac{11\tau^4}{9}\right) x^4 + \left(\frac{\tau^2}{30} + \frac{2\tau^3}{15} + \frac{\tau^4}{9}\right) x^6 \quad \text{for } l = n - 2,
\]

\[
\frac{V(x)}{\hbar \omega_0} = -\left(\frac{1}{2} + \tau - \frac{\tau^3}{6} - \frac{\tau^4}{15}\right) + \left(\frac{1}{2} - \frac{\tau^2}{2} + \frac{4\tau^4}{15}\right) x^2 + \left(\frac{\tau^2}{6} - \frac{2\tau^3}{9} - \frac{\tau^4}{6}\right) x^4
\]

\[
+ \left(\frac{\tau^2}{30} - \frac{\tau^4}{45}\right) x^6 + \left(\frac{\tau^3}{210} + \frac{\tau^4}{210}\right) x^8 \quad \text{for } l = 0,
\]

\[
V(x)_{l=1} = V(x)_{l=0} - \hbar \omega_0 (q^2 - 1)
\]

\[
\simeq V(x)_{l=0} - \hbar \omega_0 \left(2\tau + 2\tau^2 + \frac{4\tau^3}{3} + \frac{2\tau^4}{3}\right) \quad \text{for } l = 1,
\]

\[
V(x)_{l=2} = V(x)_{l=0} - \hbar \omega_0 (q^4 - q^{-2})
\]

\[
\simeq V(x)_{l=0} - \hbar \omega_0 (6\tau + 6\tau^2 + 12\tau^3 + 10\tau^4) \quad \text{for } l = 2,
\]

\[
V(x)_{l=3} = V(x)_{l=0} - \hbar \omega_0 (q^6 - 1)(1 + q^{-4})
\]

\[
\simeq V(x)_{l=0} - \hbar \omega_0 (12\tau + 12\tau^2 + 48\tau^3 + 44\tau^4) \quad \text{for } l = 3,
\]

\[
\ldots
\]

We remark that for small values of $\tau$, like the ones occurring in the previous sections, the potentials occurring for $l = n$ and $l = n - 2$ are of the form

\[
V(x) = V_0 + ax^2 - bx^4 + cx^6,
\]

with $a, b, c > 0$, while the potentials occurring for $l = 0, 1, 2, 3$ are of the form

\[
V(x) = V_0 + ax^2 + bx^4 + cx^6 + dx^8,
\]

with $a, b, c, d > 0$.

It is instructive at this point to compare these potentials with the symmetrized Woods–Saxon potential

\[
V_{SWS}(r) = -V_0 \frac{\sinh(R/a)}{\cosh(r/a) + \cosh(R/a)}, \quad 0 \leq r \leq \infty,
\]
and the “wine-bottle” symmetrized Woods–Saxon potential

\[ V_{WB}(r) = -V_0 \left(1 + \frac{w r^2}{R^2}\right) \frac{\sinh(R/a)}{\cosh(r/a) + \cosh(R/a)}, \quad 0 \leq r \leq \infty, \quad (28) \]

which have been used [26, 27] for parametrizing the Ekardt potentials [24]. In order to facilitate the comparisons, we consider the Taylor expansions of these potentials

\[ \frac{V_{SWS}(r)}{V_0 \sinh(R/a)} = -\frac{1}{1 + \cosh(R/a)} + \frac{1}{2(1 + \cosh(R/a))^2} \frac{r^2}{a^2} \]
\[ -\frac{5 - \cosh(R/a)}{24(1 + \cosh(R/a))^3} \frac{r^4}{a^4} + \frac{(\cosh(R/a))^2 - 28 \cosh(R/a) + 61 r^6}{720(1 + \cosh(R/a))^4} \frac{a^6}{R^6}, \quad (29) \]
\[ \frac{V_{WB}(r)}{V_0 \sinh(R/a)} = -\frac{1}{1 + \cosh(R/a)} + \left(\frac{1}{2(1 + \cosh(R/a))^2} - \frac{w}{1 + \cosh(R/a)} \frac{a^2}{R^2}\right) \frac{r^2}{a^2} \]
\[ -\left(\frac{5 - \cosh(R/a)}{24(1 + \cosh(R/a))^3} - \frac{w}{2(1 + \cosh(R/a))^2} \frac{a^2}{R^2}\right) \frac{r^4}{a^4} \]
\[ + \left(\frac{(\cosh(R/a))^2 - 28 \cosh(R/a) + 61}{720(1 + \cosh(R/a))^4} - \frac{w(5 - \cosh(R/a))}{24(1 + \cosh(R/a))^3} \frac{a^2}{R^2}\right) \frac{r^6}{a^6}. \quad (30) \]

The following comments are now in place:

i) The Taylor expansions of the symmetrized Woods–Saxon and the “wine-bottle” symmetrized Woods–Saxon potentials, which have been used for fitting the Ekardt potentials used for the description of metallic clusters, have the same form as the potentials corresponding to the 3-dimensional \( q \)-deformed harmonic oscillator, i.e. they contain all the even powers of the relevant variable (and no odd powers). It is therefore not surprising that the 3-dimensional \( q \)-deformed harmonic oscillator gives a good description of the magic numbers of metallic clusters.

ii) The potentials obtained through the use of perturbation theory are valid near the origin \( (x = 0) \) and for relatively low values of \( n \). They do not give information about the shape of the potential near its edges, or for very large values of \( n \). The determination of potentials which will be accurate near their edges remains an open problem. It should also be examined if these potentials possess any deeper relation to the quantum algebraic symmetry characterizing the 3-dimensional \( q \)-deformed harmonic oscillator. For example, one could check if these potentials are related to the generators of the relevant quantum algebra. The existence of such a relation also remains an open problem.

iii) For very large values of \( n \), the spectrum gets an exponential form. For example, Eq. (10) becomes (for \( \tau > 0 \))

\[ E_q(n, n) = \hbar \omega_0 \frac{e^{2\tau n} - e^{-2\tau n}}{e^{2\tau} - e^{-2\tau}} \approx \hbar \omega_0 \frac{e^{2\tau n}}{e^{2\tau} - e^{-2\tau}}. \quad (31) \]

Potentials with exponential spectra have been considered in Ref. [17], but also in this case only the form of the potential near the origin could be determined.
iv) Focusing potentials leading to $3n + l$ degeneracy of the energy levels (which has been found to describe reasonably well the magic numbers of alkali clusters \cite{38}) have been determined in Ref. \cite{38}. They have the form

$$U_3(r) = -\frac{2v}{R^4} \frac{\left(\frac{r}{R}\right)^4}{\left[\left(\frac{r}{R}\right)^6 + 1\right]^2},$$  \hspace{1cm} (32)

$$V_3(r) = E - \frac{2L_m^2}{mR_m^2} \frac{\left(\frac{r}{R_m}\right)^4}{\left[\left(\frac{r}{R_m}\right)^6 + 1\right]^2}. \hspace{1cm} (33)$$

Both of them are of the form

$$V(x) = E - A \frac{x^4}{(x^6 + 1)^2}, \hspace{1cm} (34)$$

which corresponds to a Taylor expansion of the form

$$V(x) = E - A(x^4 - 2x^{10} + 3x^{16} + \cdots). \hspace{1cm} (35)$$

We remark that this Taylor expansion bears no similarity to the Taylor expansions of the symmetrized Woods–Saxon and “wine-bottle” symmetrized Woods–Saxon potentials, since it contains only some of the even powers of the relevant variable and not all of them. Indeed, these focusing potentials are known to exhibit the “wine-bottle” feature strongly exaggerated \cite{38}, lacking in parallel the flat bottom characterizing the Woods–Saxon and Ekardt potentials. The potential $U_3(r)$ has, however, the major advantage that it reproduces quite well the edge behaviour of the Ekardt potentials \cite{38}.

8. 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 ($q = e^{i\tau}$ 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 ($q = e^{i\tau}$). (It should not be forgotten at this point that these other models have deep physical roots, while the present approach is based on symmetry arguments, which are justified a posteriori by their successful predictions.) Once the parameter is fixed, the whole spectrum is fixed and no further manipulations can be made, the choice of the energy gap $\delta$ being the only exception. However, the choice of the value of the energy gap $\delta$ does not influence the order of the energy levels, but it is just deciding which energy separations will be considered as corresponding to main magic numbers and which not. The successful prediction of the magic numbers 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) As we have already mentioned, it has been remarked [6] 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 [6] to approximate the magic numbers of alkali metal clusters with some success, and focusing potentials characterized by this degeneracy have been determined [38], but no relevant Lie symmetry could be determined [38, 39]. 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) The ability of the 3-dimensional \( q \)-deformed harmonic oscillator to reproduce correctly the magic numbers of several metal clusters is not coming as a surprise, if one considers potentials giving approximately (within the limits of perturbation theory) the same spectrum as this oscillator. The Taylor expansions of these potentials have the same form as the Taylor expansions of the symmetrized Woods–Saxon and “wine-bottle” symmetrized Woods–Saxon potentials, which successfully fit [26, 27] the Ekardt potentials [24], which characterize the structure of metal clusters.

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. Furthermore, the Taylor expansions of potentials giving approximately the same spectrum as the 3-dimensional \( q \)-deformed harmonic oscillator are found to have the same form as the Taylor expansions of the symmetrized Woods–Saxon and “wine-bottle” symmetrized Woods–Saxon potentials, which successfully fit the Ekardt potentials underlying the structure of metal clusters. Naturally, these Taylor expansions are valid near the origin. The determination of potentials which will be accurate near their edges remains an open problem. It is also an open problem the existence of any deeper relation between these potentials and the quantum algebra characterizing the 3-dimensional \( q \)-deformed harmonic oscillator, as, for example, some relation between these potentials and the generators of the quantum algebra.

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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 $\delta = 0.39$, reported between the relevant couples of energy levels.
| $n$ | $l$ | $E_q(n, l)$ | $2(2l + 1)$ | total |
|-----|-----|-------------|-------------|-------|
| 0   | 0   | 0.000       | 2           | 2     |
| 1   | 1   | 1.000       | 6           | 8     |
| 2   | 2   | 2.006       | 10          | 18    |
| 3   | 3   | 3.023       | 14          | 34    |
| 4   | 4   | 4.058       | 18          | 58    |
| 5   | 5   | 5.116       | 22          | 92    |
| 6   | 6   | 6.204       | 26          | 132   |
| 7   | 7   | 7.328       | 30          | 186   |
| 8   | 8   | 8.494       | 34          | 254   |
| 9   | 9   | 9.709       | 38          | 312   |
| 10  | 10  | 10.980      | 42          | 398   |
| 11  | 11  | 11.146      | 30          | 428   |
| 12  | 12  | 11.196      | 10          | 438   |
| 13  | 13  | 11.434      | 2           | 440   |
| 14  | 14  | 11.835      | 13          | 21.231|
| 15  | 15  | 11.835      | 13          | 21.231|
| 16  | 16  | 11.835      | 13          | 21.231|
| 17  | 17  | 11.835      | 13          | 21.231|
|     |     |             |             |       |
Table 2: Same as Table 1, but with $\hbar\omega_0 = 1$ and $q = e^r$ with $r = 0.020$. The energy gap separating different shells has been taken to be $\delta = 0.20$.

| $n$ | $l$ | $E_q(n,l)$ | $2(2l+1)$ | total | $n$ | $l$ | $E_q(n,l)$ | $2(2l+1)$ | total |
|-----|-----|------------|-----------|--------|-----|-----|------------|-----------|--------|
| 0   | 0   | 0.000      | 2         | 2      | 5   | 5   | 5.032      | 22        | 92     |
|     |     | 1.000      |           | 0.369  |      |     |            |           |        |
| 1   | 1   | 1.000      | 6         | 8      | 5   | 3   | 5.401      | 14        | 106    |
|     |     | 1.002      |           | 0.205  |      |     |            |           |        |
| 2   | 2   | 2.002      | 10        | 18     | 5   | 1   | 5.606      | 6         | 112    |
|     |     | 2.124      | 2         | 20     |      |     |            |           |        |
|     |     | 0.882      |           | 0.450  |      |     |            |           |        |
|     |     |            | 6         | 6      | 6.056 | 26   | 138        |           |        |
|     |     |            |           | 0.453  |      |     |            |           |        |
| 3   | 3   | 3.006      | 14        | 34     | 6   | 4   | 6.509      | 18        | 156    |
|     |     | 0.205      |           | 0.286  |      |     |            |           |        |
|     |     |            | 6         | 2      | 6.795 | 10   | 166        |           |        |
|     |     |            |           | 6.918  | 2     | 168  |           |           |        |
|     |     |            |           | 0.287  | 7     | 7.090 | 30        | 198      |        |
|     |     |            |           | 0.536  | 7     | 7.626 | 22        | 220      |        |
| 4   | 2   | 4.303      | 10        | 68     | 7   | 5   | 7.626      | 22        | 220    |
|     |     | 4.425      | 2         | 70     |      |     |            |           |        |
|     |     | 0.607      |           | 0.369  |      |     |            |           |        |
Table 3: Same as Table 1, but with $\hbar \omega_0 = 1$ and $q = e^{\tau}$ with $\tau = 0.050$. The energy gap separating different shells has been taken to be $\delta = 0.38$.

| $n$ | $l$ | $E_q(n,l)$ | $2(2l+1)$ | total | $n$ | $l$ | $E_q(n,l)$ | $2(2l+1)$ | total |
|-----|-----|------------|-----------|-------|-----|-----|------------|-----------|-------|
| 0   | 0   | 0.000      | 2         | 2     | 11  | 11  | 13.334     | 46        | 486   |
|     |     | 1.000      |           |       |     |     | 0.389      |           |       |
| 1   | 1   | 1.000      | 6         | 8     | 9   | 5   | 13.723     | 22        | 508   |
|     |     | 1.010      |           |       | 10  | 8   | 14.044     | 34        | 542   |
| 2   | 2   | 2.010      | 10        | 18    |     |     | 0.658      |           |       |
| 2   | 0   | 2.327      | 2         | 20    | 9   | 3   | 14.702     | 14        | 556   |
|     |     | 0.713      |           |       | 12  | 12  | 15.069     | 50        | 606   |
| 3   | 3   | 3.040      | 14        | 34    | 9   | 1   | 15.233     | 6         | 612   |
|     |     | 0.531      |           |       |     |     | 0.540      |           |       |
| 3   | 1   | 3.571      | 6         | 40    | 10  | 6   | 15.773     | 26        | 638   |
|     |     | 0.530      |           |       | 11  | 9   | 15.971     | 38        | 676   |
| 4   | 4   | 4.101      | 18        | 58    |     |     | 0.985      |           |       |
|     |     | 0.751      |           |       | 13  | 13  | 16.956     | 54        | 730   |
| 4   | 2   | 4.852      | 10        | 68    | 10  | 4   | 16.989     | 18        | 748   |
| 4   | 0   | 5.168      | 2         | 70    |     |     | 0.751      |           |       |
| 5   | 5   | 5.202      | 22        | 92    | 10  | 2   | 17.740     | 10        | 758   |
|     |     | 0.979      |           |       | 11  | 7   | 17.981     | 30        | 788   |
| 5   | 3   | 6.181      | 14        | 106   | 10  | 0   | 18.056     | 2         | 790   |
| 6   | 6   | 6.356      | 26        | 132   | 12  | 10  | 18.057     | 42        | 832   |
| 5   | 1   | 6.712      | 6         | 138   |     |     | 0.954      |           |       |
|     |     | 0.860      |           |       | 14  | 14  | 19.011     | 58        | 890   |
| 6   | 4   | 7.572      | 18        | 156   |     |     | 0.435      |           |       |
| 7   | 7   | 7.573      | 30        | 186   | 11  | 5   | 19.446     | 22        | 912   |
|     |     | 0.750      |           |       |     |     | 0.878      |           |       |
| 6   | 2   | 8.323      | 10        | 196   | 13  | 11  | 20.324     | 46        | 958   |
| 6   | 0   | 8.639      | 2         | 198   | 12  | 8   | 20.368     | 34        | 992   |
| 8   | 8   | 8.866      | 34        | 232   | 11  | 3   | 20.424     | 14        | 1006  |
| 7   | 5   | 9.038      | 22        | 254   |     |     | 0.531      |           |       |
|     |     | 0.979      |           |       | 11  | 1   | 20.955     | 6         | 1012  |
| 7   | 3   | 10.017     | 14        | 268   | 15  | 15  | 21.257     | 62        | 1074  |
| 9   | 9   | 10.248     | 38        | 306   |     |     | 0.840      |           |       |
| 7   | 1   | 10.548     | 6         | 312   | 12  | 6   | 22.097     | 26        | 1100  |
| 8   | 6   | 10.595     | 26        | 338   |     |     | 0.697      |           |       |
|     |     | 1.137      |           |       | 14  | 12  | 22.794     | 50        | 1150  |
| 10  | 10  | 11.732     | 42        | 380   | 13  | 9   | 22.960     | 38        | 1188  |
| 8   | 4   | 11.811     | 18        | 398   | 12  | 4   | 23.313     | 18        | 1206  |
|     |     | 0.447      |           |       |     |     | 0.403      |           |       |
| 9   | 7   | 12.258     | 30        | 428   | 16  | 16  | 23.716     | 66        | 1272  |
| 8   | 2   | 12.562     | 10        | 438   | 12  | 2   | 24.064     | 10        | 1282  |
| 8   | 0   | 12.878     | 2         | 440   | 12  | 0   | 24.381     | 2         | 1284  |
|     |     | 0.456      |           |       |     |     | 0.589      |           |       |
|     |     | 13         | 7         | 24.970  | 30  | 1314 |


Table 4: Magic numbers provided by the 3-dimensional $q$-deformed harmonic oscillator (Table 1), reported in column 1, are compared to the experimental data for Na clusters by Martin et al. [6] (column 2), Bjørnholm et al. [7] (column 3), Knight et al. [8] (column 4), and Pedersen et al. [9] (column 5), as well as to the experimental data for Li clusters by Bréchignac et al. ([10] in column 6, [11] in column 7). The magic numbers provided [5] by the (non-deformed) 3-dimensional harmonic oscillator (column 10), the square well potential (column 9) and a rounded square well potential intermediate between the previous two (column 8) are also shown for comparison. See text for discussion.

| th. exp. Na | exp. Na | exp. Na | exp. Na | exp. Li | exp. Li | th. int. | sq. well | h. osc. |
|---|---|---|---|---|---|---|---|---|
| present Tab. 1 Ref.[6] | Ref.[7] | Ref.[8] | Ref.[9] | Ref.[10] | Ref.[11] | Ref.[5] | Ref.[5] | Ref.[5] |
| 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 |
| 8 | 8 | 8 | 8 | 8 | 8 | 8 | 8 |
| (18) | 18 | | | | 18 | 18 |
| 20 | 20 | 20 | 20 | 20 | 20 | 20 | 20 |
| 34 | 34 | | | | 34 | 34 |
| 40 | 40 | 40 | 40 | 40 | 40 | 40 | 40 |
| 58 | 58 | 58 | 58 | 58 | 58 | 68,70 | 68 | 70 |
| 92 | 92 | 92 | 92 | 92 | 93 | 92 | 92 | 90,92 |
| 138 | 138 | 138 | 138 | 134 | 138 | 138 | 138 | 132,138 |
| 198 | 198±2 | 196 | 198 | 191 | 198 | 156 | 156 | 168 |
| 254 | 260±4 | | | | 258 | | | |
| 268 | 263±5 | 264 | 262 | | | | | |
| 338 | 341±5 | 344±4 | 344 | 342 | 336 | | | |
| 440 | 443±5 | 440±2 | 442 | 442 | 440 | | | |
| 556 | 557±5 | 558±8 | 554 | 552 | 546 | | | |
| 676 | | | | | 680 | | | |
| 694 | 700±15 | | | | 695 | 710 | | |
| 832 | 840±15 | 800 | 822 | 820 | | | | |
| 912 | | | | | 902 | | | |
| 1012 | 1040±20 | 970 | 1025 | 1065 | | | | |
| 1100 | | | | | 1120 | | | |
| 1206 | 1220±20 | | | | | | | |
| 1284 | | | | | 1297 | 1270 | | |
| 1314 | | | | | 1310 | | | |
| 1410 | 1430±20 | | | | | | | |
| 1502 | | | | | 1500 | 1510 | | |

20
Table 5: Magic numbers provided by the 3-dimensional $q$-deformed harmonic oscillator (Table 1), reported in column 1, are compared to the experimental data for Na clusters by Martin et al. [6] (column 2), and Pedersen et al. [9] (column 3), as well as to the experimental data for Li clusters by Bréchignac et al. [10] (column 4) and to the theoretical predictions of various jellium model calculations reported by Martin et al. [6] (column 5), Bjørnholm et al. [7] (column 6), Brack [2] (column 7), Bulgac and Lewenkopf [42] (column 8), the theoretical predictions of Woods–Saxon and “wine bottle” potentials reported by Nishioka et al. [43] (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. [6] (column 10). See text for discussion.

| th. | exp. | exp. | exp. | th. | th. | th. | th. | th. | th. |
|-----|------|------|------|-----|-----|-----|-----|-----|-----|
| present | Na   | Na   | Li   | jell. | jell. | jell. | jell. | WS   | $3n + l$ |
| Tab. 1 | Ref.[6] | Ref.[9] | Ref.[10] | Ref.[6] | Ref.[7] | Ref.[2] | Ref.[42] | Ref.[43] | Ref.[6] |
| 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 |
| 8 | 8 | 8 | 8 | 8 | 8 | 8 | 8 | 8 | 8 |
| (18) | 18 | 18 | (20) | 20 | 20 | 20 | 20 | 18 | 18 |
| 20 | 20 | 20 | 20 | 20 | 20 | 20 | 20 | 20 | 20 |
| 34 | 34 | 34 | 34 | 34 | 34 | 34 | 34 | 34 | 34 |
| 40 | 40 | 40 | (40) | 40 | 40 | 40 | 40 | 40 | 40 |
| 58 | 58 | 58 | 58 | 58 | 58 | 58 | 58 | 58 | 58 |
| 92 | 90,92 | 92 | 92 | 92 | 92 | 92 | 92 | 92 | 90 |
| 138 | 138 | 138 | 134 | 134 | 138 | 138 | 138 | 138 | 132 |
| 198 | 198±2 | 198 | 191 | (196) | 196 | 196 | 196 | 198 | 198 |
| 254 | 254 | 254 | 254 | 254 | 254 | 254 | 254 | 254 | 254 |
| 268 | 263±5 | 264 | 262 | (268) | 268 | 268 | 268 | 268 | 268 |
| 338 | 341±5 | 344 | 342 | 338(356) | 338 | 338 | 338 | 338 | 332 |
| 440 | 443±5 | 442 | 442 | 440 | 440 | 438,440 | 440 | 440 | 428 |
| 556 | 557±5 | 554 | 552 | 562 | 562 | 556 | 556 | 556 | 562 |
| 676 | 680 | 676 | 676 | 676 | 676 | 676 | 676 | 676 | 670 |
| 694 | 700±15 | 695 | 704 | | | | | 694 | 694 |
| 758 | 748 | | | | | | | | 758 |
| 832 | 840±15 | 800 | 822 | 852 | 832 | 832 | 832 | 832 | 820 |
| 912 | 902 | | | | | | | | 912 |
| 1012 | 1040±20 | 970 | 1025 | 1074 | 1074 | 1012 | 1012 | 990 | 990 |
| 1100 | 1120 | | | | | | | | 1100 |
| 1206 | 1220±20 | | | | | | | | 1216 |
| 1284 | 1297 | 1284 | 1284 | 1284 | 1284 | 1284 | 1284 | 1284 | 1284 |
| 1314 | 1310 | | | | | | | 1314 | 1314 |
| 1410 | 1430±20 | | | | | | | | 1398 |
| 1502 | 1500 | 1502 | 1502 | 1502 | 1502 | 1502 | 1502 | 1502 | 1516 |
Table 6: Magic numbers provided by the 3-dimensional $q$-deformed harmonic oscillator (Table 1), reported in column 1, are compared to the experimental data for clusters of Li [10] (column 2), Na [6] (column 3), K [12] (column 4), Rb [13] (column 5), Cs [7,14] (column 6), Cu [16] (column 7), Ag ([18] in column 8, [16] in column 9), and Au [16] (column 10). See text for discussion.

| th. exp. | exp. Li | exp. Na | exp. K | exp. Rb | exp. Cs | exp. Cu | exp. Ag | exp. Ag | exp. Au |
|---------|---------|---------|--------|---------|--------|--------|--------|--------|--------|
| present | Ref.[10] | Ref.[6] | Ref.[12] | Ref.[13] | Ref.[7,14] | Ref.[16] | Ref.[18] | Ref.[16] | Ref.[16] |
| 2       | 2       | 2       | 2      | 2       | 2      | 2      | 2      | 2      | 2      |
| 8       | 8       | 8       | 8      | 8       | 8      | 8      | 8      | 8      | 8      |
| (18)    | 18      | 18      | 18     | 18      | 18     | 18     | 18     | 18     | 18     |
| 20      | 20      | 20      | 20     | 20      | 20     | 20     | 20     | 20     | 20     |
| 34      | 34      | 34      | 34     | 34      | 34     | 34     | 34     | 34     | 34     |
| 40      | 40      | 40      | 40     | 40      | 40     | 40     | 40     | (40)   | 40     |
| 58      | 58      | 58      | 58     | 58      | 58     | 58     | 58     | 58     | 58     |
| 92      | 93      | 90,92   | 92     | 92      | 92     | 92     | 92     | 92     | 92     |
| 138     | 134     | 138     | 138    | 138     | 138    | 138    | 138    | 138    | 138    |
| 198     | 191     | 198±2   | 198±2  | 198±2   | 198±2  | 198±2  | 198±2  | 198±2  | 198±2  |
| 254     |         |         |        |         |        |        |        |        |        |
| 268     | 262     | 263±5   | 263±5  | 268±5   | 268±5  | 268±5  | 268±5  | 268±5  | 268±5  |
| 338     | 342     | 341±5   | 341±5  | 338±15  | 338±15 | 338±15 | 338±15 | 338±15 | 338±15 |
| 440     | 442     | 443±5   | 443±5  | 440±15  | 440±15 | 440±15 | 440±15 | 440±15 | 440±15 |
| 556     | 552     | 557±5   | 557±5  |         |         |         |         |         |         |
| 676     |         |         |        |         |         |         |         |         |         |
| 694     | 695     | 700±15  | 700±15 |         |         |         |         |         |         |
| 832     | 822     | 840±15  | 840±15 |         |         |         |         |         |         |
| 912     | 902     |         |        |         |         |         |         |         |         |
| 1012    | 1025    | 1040±20 | 1040±15|         |         |         |         |         |         |
| 1100    |         |         |        |         |         |         |         |         |         |
| 1206    |         | 1220±20 |         |         |         |         |         |         |         |
| 1284    |         | 1297    |         |         |         |         |         |         |         |
| 1314    |         |         |        |         |         |         |         |         |         |
| 1410    |         | 1430±20 |         |         |         |         |         |         |         |
| 1502    |         |         |        |         |         |         |         |         |         |
Table 7: Magic numbers provided by the 3-dimensional $q$-deformed harmonic oscillator of Table 1 with energy gap $\delta = 0.26$ (column 1) and of Table 2 (column 2), are compared to the experimental data for Zn clusters [19] (column 4) and Cd clusters [19] (column 5), as well as to the theoretical predictions of a potential intermediate between the simple harmonic oscillator and the square well potential [19] (column 3). In addition, the magic numbers provided by the 3-dimensional $q$-deformed harmonic oscillator of Table 3 (reported in column 6) are compared to the experimental data for Al [20] (column 7) and In [20] (column 8). See text for discussion.

| th. | th. | th. | exp. | exp. | th. | exp. | exp. |
|-----|-----|-----|------|------|-----|------|------|
| present | present | Ref.[19] | Ref.[19] | Ref.[19] | present | Al | In |
| Tab. 1 | Tab. 2 | Ref.[19] | Ref.[19] | Ref.[19] | Tab. 3 | Ref.[20] | Ref.[20] |
| 2 | 2 | 2 | 2 | 8 | 8 | 8 |
| 20 | 20 | 20 | 20 | 20 | 20 | 20 |
| 34 | 34 | 34 | (36) | (36) | 34 |
| 40 | 40 | 40 | 40 | 40 | 40 | 40 |
| 58 | 58 | 58 | 56 | 56 | 58 |
| 68 | (60) | (60) |
| 70 | 70 | 70 | 70 | 70 |
| (80) | (80) |
| (82) |
| 92 | 92 | 92 | 92 | 92 | 92 | 92 |
| 106 | 106 | 102 | 108 | 108 |
| 112 | 112 | (114) |
| (120) | (120) |
| 138 | 138 | 138 | 138 | 138 | 138 | 138 |

164
186
198
198
254
252
338
336
398
440
438
486
468±6
542
534±6
612
594±6
676
688±6
748
742±6
832
832±10
890
912
918±10
1006
1000±10
1074
1100
1112±10
1206
1224±10