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

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Magic numbers predicted by a three-dimensional *q*-deformed harmonic oscillator with $\mathrm{u}_q(3)\supset\mathrm{so}_q(3)$ symmetry are compared to experimental data for atomic clusters of alkali metals (Li, Na, K, Rb, and Cs), noble metals (Cu, Ag, and Au), divalent metals (Zn and Cd), and trivalent metals (Al and 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 three-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 $\mathrm{u}_q(3)$, which is a nonlinear extension of the u(3) symmetry of the spherical (three-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 three-dimensional *q*-deformed harmonic oscillator are found to be similar to the Taylor expansions of the symmetrized Woods-Saxon potential and wine bottle symmetrized Woods-Saxon potential, which are known to provide successful fits of the Ekardt potentials.

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I. INTRODUCTION

Metal clusters have recently been the subject of many investigations (see Refs. [1–4] 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 [6–9], Li [10,11], K [12], Rb [13], and Cs [7,14,15]), noble metals (Cu [16,17], Ag [16,18], and Au [16]), and divalent metals of the IIB group (Zn and Cd) [19], trivalent metals of the III group (Al and 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 ''wine bottle'' type [26,27]. 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 was given in terms of a scheme intermediate between the level scheme of the three-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 recently been investigated in the 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 τ being real) or more rapidly (for *q* being real, i.e., $q=e^{\tau}$, with τ being real) in comparison to the equidistant spectrum of the usual harmonic oscillator [32], 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 three-dimensional harmonic oscillator was constructed [35], taking advantage of the $\mathrm{u}_q(3)\supset\mathrm{so}_q(3)$ symmetry [36,37]. The spectrum of this three-dimensional *q*-deformed harmonic oscillator was 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 model of Refs. [22,23] 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 three-dimensional *q*-deformed harmonic oscillator can reproduce the magic numbers of simple metallic clusters and, if this this is possible, to determine potentials giving the same spectrum as this oscillator and compare them with the symmetrized Woods-Saxon potential and wine bottle symmetrized Woods-Saxon potential, 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 was inspired by the fact that degenerate energy levels in the hydro-

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gen 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 three-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 was used [6] to approximate the magic numbers of alkali-metal clusters with some success, and focusing potentials characterized by this degeneracy were determined [38], but no relevant Lie symmetry could be determined [38,39].

In Sec. II the three-dimensional q-deformed harmonic oscillator will be briefly described, while in Sec. III 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 (the jellium model, the Woods-Saxon and ‘‘wine bottle’’ potentials, and a classification scheme using the $3n+l$ pseudo-quantum-number). Additional comparisons of magic numbers predicted by the three-dimensional q-deformed harmonic oscillator to experimental data and to the results of other theoretical approaches will be made in Sec. IV (for other alkali-metal clusters and noble-metal clusters), Sec. V (for divalent group-IIB metal clusters), and Sec. VI (for trivalent group-III metal clusters), while in Sec. VII potentials giving approximately the same spectrum as the three-dimensional q-deformed harmonic oscillator will be determined, and subsequently compared to the symmetrized Woods-Saxon potential and ‘‘wine bottle’’ symmetrized Woods-Saxon potential. Finally, Sec. VIII will contain a discussion of the present results and plans for further work.

II. THREE-DIMENSIONAL *q*-DEFORMED HARMONIC OSCILLATOR

The space of the three-dimensional q-deformed harmonic oscillator consists of completely symmetric irreducible representations of the quantum algebra $\mathrm{u}_q(3)$. In this space a deformed angular momentum algebra, $\mathrm{so}_q(3)$, can be defined [35]. The Hamiltonian of the three-dimensional q-deformed harmonic oscillator is defined so that it satisfies the following requirements.

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

(b) It conserves the number of bosons, in terms of which the quantum algebras $\mathrm{u}_q(3)$ and $\mathrm{so}_q(3)$ are realized.

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

It was proved [35] that the Hamiltonian of the three-dimensional q-deformed harmonic oscillator satisfying the above requirements takes the form

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

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

$$[x]=\frac{q^x-q^{-x}}{q-q^{-1}} \tag{2}$$

is the definition of q numbers and q operators.

The energy eigenvalues of the three-dimensional q-deformed harmonic oscillator are then [35]

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

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

For small values of the deformation parameter τ (where $q=e^\tau$), one can expand Eq. (3) in powers of τ, obtaining [35]

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

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)

$$V=\frac{1}{2}\hbar\omega\rho^2-\hbar\omega\kappa'(\mathbf{L}^2-\langle\mathbf{L}^2\rangle_N),\quad \rho=r\sqrt{\frac{M\omega}{\hbar}}, \tag{5}$$

where

$$\langle\mathbf{L}^2\rangle_N=\frac{N(N+3)}{2}. \tag{6}$$

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 [35] that the spectrum of the three-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 resemble the Woods-Saxon potential.

The level scheme of the three-dimensional q-deformed harmonic oscillator (for $\hbar\omega_0=1$ and $\tau=0.038$) is given in Table I, 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 δ, is larger

TABLE I. Energy spectrum $E_q(n,l)$ of the three-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 pairs 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			0.397		
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**			0.603		
		0.638			10	4	14.757	18	**694**
4	4	4.058	18	**58**			0.449		
		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			0.884		
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			0.559		
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			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
		0.781			14	10	21.360	42	**1410**
							0.475		
					13	5	21.835	22	1432
					17	17	22.119	70	**1502**
							0.441		
					13	3	22.560	14	1516

TABLE II. Same as Table I, but with $\hbar\omega_0=1$ and $q=e^{\tau}$ with $\tau=0.020$. 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	0	2.124	2	**20**			0.450		
		0.882			6	6	6.056	26	**138**
3	3	3.006	14	**34**			0.453		
		0.205			6	4	6.509	18	**156**
3	1	3.211	6	**40**			0.286		
		0.805			6	2	6.795	10	166
4	4	4.016	18	**58**	6	0	6.918	2	168
		0.287			7	7	7.090	30	**198**
4	2	4.303	10	68			0.536		
4	0	4.425	2	**70**	7	5	7.626	22	**220**
		0.607					0.369		

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 three-dimensional *q*-deformed harmonic oscillator are given in Table II (for $\tau=0.020$ and an energy gap $\delta=0.20$) and in Table III (for $\tau=0.050$ and an energy gap $\delta=0.38$). The following remarks are now in place.

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

(ii) A rapid change of the magic numbers as a function of τ occurs when τ takes negative values, but this case is irrelevant to the contents of the present work.

(iii) Magic numbers are influenced nore drastically by the value of the energy gap δ. If in the spectrum obtained for a given value of the parameter τ the energy separation between two successive levels is only slightly smaller than the energy gap δ, this can be considered as an indication of the presence of a ‘‘secondary’’ magic number. (See the end of Sec. III for specific examples.)

III. SODIUM AND LITHIUM CLUSTERS

The magic numbers provided by the three-dimensional *q*-deformed harmonic oscillator in Table I are compared to available experimental data for Na clusters [6–9] and Li clusters [10,11] in Table IV (columns 2–7). Some preliminary results concerning Na clusters were already given earlier in Ref. [40]. 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 [6].

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

(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 IV the predictions of three simple theoretical models [5] [nondeformed three-dimensional harmonic oscillator (column 10), a square-well potential (column 9), and a rounded square-well potential (intermediate between the previous two, column 8)] are also reported for comparison. It is clear that the predictions of the nondeformed three-dimensional harmonic oscillator are in agreement with the experimental data only up to magic number 40, while the other two models correctly give a few more magic numbers (58, 92, and 138), although they already fail by predicting magic numbers at 68, 70, 106, 112, and 156, which are not observed. It should be noted 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 [41], this assumption being applicable under conditions not favoring a 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 IV, can be made in Table V, where magic numbers predicted by various jellium model calculations (columns 5–8 [6,7,2,42]), and Woods-Saxon and wine bottle potentials (column 9, [43]), as well as by a classification scheme using the $3n+l$ pseudo-quantum-number (column 10 [6]) are reported. The following observations can be made:

(i) All magic numbers predicted by the three-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 and 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. [43] predict a magic number at 68, for which no experimental support exists. The present scheme avoids problems at these numbers. It should be noted, however, that in the cases of 186 and 542 the energy gaps following them in the present scheme are 0.329 and 0.325, respectively (see Table I), 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

TABLE III. Same as Table I, 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**

qualitatively remark that 186 and 542 are ‘‘built into’’ the present scheme as ‘‘secondary’’ (not very pronounced) magic numbers.

IV. 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 ([18] in column 8 and [16] in column 9), Au ([16], column 10)] are reported in Table VI, along with the theoretical predictions of the three-dimensional q-deformed harmonic oscillator given in Table I. The following comments apply.

(i) In the cases of Rb [13], Cu [16], Ag [16], and Au [16], what is seen experimentally is cations of the type Rb_N^+, Cu_N^+, Ag_N^+, and Au_N^+, which contain N atoms each, but $N-1$ electrons. The magic numbers reported in Table VI are

TABLE IV. Magic numbers provided by the three-dimensional q-deformed harmonic oscillator (Table I), 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.* (Ref. [10] in column 6, and Ref. [11] in column 7). The magic numbers provided [5] by the (non-deformed) three-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.

Theor. present Table I	Expt. Na Ref. [6]	Expt. Na Ref. [7]	Expt. Na Ref. [8]	Expt. Na Ref. [9]	Expt. Li Ref. [10]	Expt. Li Ref. [11]	Theor. int. Ref. [5]	Theor. sq. well Ref. [5]	Theor. h. osc. 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	40
58	58	58	58	58		58	58	58	
							68,70	68	70
92	90,92	92	92	92	93	92	92	90,92	
							106,112	106	112
138	138	138		138	134	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			

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 three-dimensional q-deformed harmonic oscillator of Table I. The limited data on K, Rb, Cu, and Au also agree with the magic numbers of Table I.

V. DIVALENT METALS OF THE IIB GROUP

For these metals the quantities determined experimentally [19] are numbers of atoms exhibiting ‘‘magic’’ behavior. 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 [19] are reported in Table VII (in columns 4 and 5, respectively), along with the magic numbers predicted by the three-dimensional q-deformed harmonic oscillator for two different parameter values (given in Tables I and II, 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 [19] 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 Ref. [1].

(ii) In column 1 of Table VII, magic numbers of the three-dimensional q-deformed harmonic oscillator with $\tau = 0.038$

TABLE V. Magic numbers provided by the three-dimensional q-deformed harmonic oscillator (Table I), 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), Bjϕrnholm *et al.* [7] (column 6), Brack [2] (column 7), and Bulgac and Lewenkopf [42] (column 8); the theoretical predictions of Woods-Saxon and ''wine bottle'' potentials reported by Nishioka *et al.* [43] (column 9); and 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.

Theor. present Table I	Expt. Na Ref. [6]	Expt. Na Ref. [9]	Expt. Li Ref. [10]	Theor. jell. Ref. [6]	Theor. jell. Ref. [7]	Theor. jell. Ref. [2]	Theor. jell. Ref. [42]	Theor. WS Ref. [43]	Theor. $3n+l$ Ref. [6]
2	2			2	2	2		2	2
8	8			8	8	8		8	8
(18)	18			18	18				18
20	20			(20)	20	20		20	
34	34			34	34	34	34		34
40	40	40		(40)	40			40	
58	58	58		58	58	58	58	58	58
								68	
92	90,92	92	93	92	92	92	92	92	90
138	138	138	134	134	138	138	138	138	132
				186	186	186	186		186
198	198±2	198	191	(196)	196			198	
254				254	254	254	254	254	252
268	263±5	264	262	(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
						542	542		540
556	557±5	554	552	562	556	556	556	562	
676		680			676	676	676		670
694	700±15		695	704				694	
						758	748		
832	840±15	800	822	852	832	832	832	832	820
912			902			912	912		
1012	1040±20	970	1025			1074	1074	1012	990
1100		1120				1100	1100	1100	
1206	1220±20							1216	1182
1284			1297			1284	1284		
1314		1310						1314	
1410	1430±20								1398
1502		1500				1502	1502	1516	

and energy gaps larger than 0.26 are reported. Decreasing the energy gap δ, considered as separating different shells from 0.39 (used in Table I) to 0.26 (used in Table VII), has as the result that the numbers 70 and 106 become magic, in close agreement with the experimental data. Similar but even better results are obtained from the three-dimensional q-deformed harmonic oscillator of Table II, reported in column 2 of Table VII. This oscillator is characterized by $\tau=0.020$, while the energy gap δ 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 therefore remark that the general agreement between the results given by the three-dimensional q-deformed harmonic oscillator and the experimental data is not sensitively dependent on the parameter value, but, in contrast, quite different parameter values ($\tau=0.038$ and 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.

VI. TRIVALENT METALS OF THE III GROUP

Magic numbers of electrons for the trivalent metals Al and In [20] are reported in Table VII (in columns 7 and 8,

TABLE VI. Magic numbers provided by the three-dimensional q-deformed harmonic oscillator (Table I), 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 (Ref. [18] in column 8, and Ref. [16] in column 9), and Au [16] (column 10). See text for discussion.

Theor. present Table I	Expt. Li Ref. [10]	Expt. Na Ref. [6]	Expt. K Ref. [12]	Expt. Rb Ref. [13]	Expt. Cs Ref. [7,14]	Expt. Cu Ref. [16]	Expt. Ag Ref. [18]	Expt. Ag Ref. [16]	Expt. Au Ref. [16]
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	34	34	34	34
40		40	40	40	40	40	(40)	40	
58		58	58		58	58	58	58	58
92	93	90,92			92	92	92	92	92
138	134	138			138	138	138	138	138
198	191	198 ± 2			198 ± 2		186 ± 4	198	
254									
268	262	263 ± 5			263 ± 5		268 ± 5		
338	342	341 ± 5			341 ± 5		338 ± 15		
440	442	443 ± 5			443 ± 5		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									

respectively), along with the predictions of the three-dimensional q-deformed harmonic oscillator of Table III (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 the 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 III provides the magic numbers reported in column 6 of Table VII. 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, and 1074, which are not seen in the experiment reported in column 7.

VII. POTENTIALS CORRESPONDING TO THE THREE-DIMENSIONAL *q*-DEFORMED HARMONIC OSCILLATOR

As we have seen in previous sections, the three-dimensional q-deformed harmonic oscillator successfully describes 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 the symmetrized Woods-Saxon potential and wine bottle symmetrized Woods-Saxon potential [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

TABLE VII. Magic numbers provided by the three-dimensional q-deformed harmonic oscillator of Table I with energy gap $\delta = 0.26$ (column 1) and of Table II (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 three-dimensional q-deformed harmonic oscillator of Table III (reported in column 6) are compared to the experimental data for Al [20] (column 7) and In [20] (column 8). See text for discussion.

Theor. present Table I	Theor. present Table II	Theor. Ref. [19]	Expt. Zn Ref. [19]	Expt. Cd Ref. [19]	Theor. present Table III	Expt. Al Ref. [20]	Expt. In Ref. [20]
2	2				2		
8	8				8		
20	20	20	20	20	20		
34	34	34	(36)	(36)	34		
40	40	40	40	40	40		
58	58	58	56	56	58		
			(60)	(60)			
		68	(64)	(64)			
70	70	70	70	70			
			(80)	(80)			
			(82)				
92	92	92	92	92	92		
106	106	102	108	108			
	112	112	(114)				
			(120)	(120)			
138	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	

the three-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

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

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

$$\begin{aligned} E = {}& \epsilon_0 + \kappa + 3\lambda + 15\mu + 105\xi + (2\kappa + 6\lambda + 40\mu + 280\xi)n \\ & + (6\lambda + 30\mu + 350\xi)n^2 + (20\mu + 140\xi)n^3 + 70\xi n^4. \end{aligned} \tag{9}$$

The second term in Eq. (8) corresponds to the usual harmonic oscillator. For appropriate values of the numerical coefficients κ, λ, μ, and ξ, the rest of the terms can be considered as perturbations to the harmonic oscillator.

It is clear that this method can be applied in cases in which the spectrum under study depends on only one quantum number, the number of excitation quanta *n*. In the case of the three-dimensional *q*-deformed harmonic oscillator [Eq. (3)], however, the spectrum depends on an additional quantum number: the angular momentum *l*. One way out of this is to determine an *l*-dependent equivalent potential, as it is done in several branches of physics [45,46]. In order to do this, for each possible value of l ($l=n, n-2, n-4, \ldots 1$, or 0 [see Eq. (3)] one determines the energy as a function of *n* only, and then calculates the corresponding potential.

In the case of the three-dimensional *q*-deformed harmonic oscillator, the energy spectrum $E_q(n,l)$ for the various possible values of the angular momentum l ($l=n$, $n-2$, $n-4,\ldots,1$ or 0) can be put into the forms

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

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

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

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

$$\ldots$$

$$\begin{aligned}E_q(n,3)&=\hbar\omega_0(q^8[[n-3]]_{q^2}+q^{-4}[[5]]_{q^2}\\&\quad -q^{-2}[[3]]_{q^2}+1)\\&=E_q(n,0)-\hbar\omega_0(q^6-1)(1+q^{-4}) \quad \text{for } l=3,\end{aligned} \tag{14}$$

$$\begin{aligned}E_q(n,2)&=\hbar\omega_0(q^6[[n-2]]_{q^2}+q^{-2}[[3]]_{q^2}-1)\\&=E_q(n,0)-\hbar\omega_0(q^4-q^{-2}) \quad \text{for } l=2,\end{aligned} \tag{15}$$

$$\begin{aligned}E_q(n,1)&=\hbar\omega_0(q^4[[n-1]]_{q^2}+1)\\&=E_q(n,0)-\hbar\omega_0(q^2-1) \quad \text{for } l=1,\end{aligned} \tag{16}$$

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

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

$$[[n]]_q=\frac{q^n-1}{q-1}, \tag{18}$$

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

We then consider the Taylor expansions for these energy expressions. By comparing these to Eq. (9), and equating the coefficients of the various powers of n (up to n^4), in each case we determine the coefficients κ, λ, μ, and ξ. Substituting these coefficients into Eq. (8), for each case we determine the corresponding potential, keeping terms up to τ^4 (where $q=e^{\tau}$). The first few cases are

$$\begin{aligned}\frac{V(x)_{l=n}}{\hbar\omega_0}&=-\left(\frac{1}{2}-\frac{\tau^2}{2}+\frac{4\tau^4}{15}\right)+\left(\frac{1}{2}-\frac{\tau^2}{2}+\frac{4\tau^4}{15}\right)x^2\\&\quad-\left(\frac{\tau^2}{6}-\frac{\tau^4}{9}\right)x^4+\left(\frac{\tau^2}{30}-\frac{\tau^4}{45}\right)x^6 \quad \text{for } l=n,\end{aligned} \tag{19}$$

$$\begin{aligned}\frac{V(x)_{l=n-2}}{\hbar\omega_0}&=-\left(\frac{1}{2}+4\tau+\frac{7\tau^2}{2}+\frac{8\tau^3}{3}+\frac{8\tau^4}{5}\right)\\&\quad+\left(\frac{1}{2}+2\tau+\frac{3\tau^2}{2}+\frac{10\tau^3}{3}+\frac{44\tau^4}{15}\right)x^2\\&\quad-\left(\frac{\tau^2}{6}+\frac{4\tau^3}{3}+\frac{11\tau^4}{9}\right)x^4\\&\quad+\left(\frac{\tau^2}{30}+\frac{2\tau^3}{15}+\frac{\tau^4}{9}\right)x^6 \quad \text{for } l=n-2,\end{aligned} \tag{20}$$

$$\ldots$$

$$\begin{aligned}\frac{V(x)_{l=0}}{\hbar\omega_0}&=-\left(\frac{1}{2}+\frac{\tau}{2}-\frac{\tau^3}{6}-\frac{\tau^4}{15}\right)+\left(\frac{1}{2}-\frac{\tau^2}{2}+\frac{4\tau^4}{15}\right)x^2\\&\quad+\left(\frac{\tau}{6}-\frac{2\tau^3}{9}-\frac{\tau^4}{6}\right)x^4+\left(\frac{\tau^2}{30}-\frac{\tau^4}{45}\right)x^6\\&\quad+\left(\frac{\tau^3}{210}+\frac{\tau^4}{210}\right)x^8 \quad \text{for } l=0,\end{aligned} \tag{21}$$

$$\begin{aligned}V(x)_{l=1}&=V(x)_{l=0}-\hbar\omega_0(q^2-1)\\&\simeq V(x)_{l=0}-\hbar\omega_0\left(2\tau+2\tau^2+\frac{4\tau^3}{3}+\frac{2\tau^4}{3}\right) \quad \text{for } l=1,\end{aligned} \tag{22}$$

$$\begin{aligned}V(x)_{l=2}&=V(x)_{l=0}-\hbar\omega_0(q^4-q^{-2})\\&\simeq V(x)_{l=0}-\hbar\omega_0(6\tau+6\tau^2+12\tau^3+10\tau^4) \quad \text{for } l=2,\end{aligned} \tag{23}$$

$$\begin{aligned}V(x)_{l=3}&=V(x)_{l=0}-\hbar\omega_0(q^6-1)(1+q^{-4})\\&\simeq V(x)_{l=0}-\hbar\omega_0(12\tau+12\tau^2+48\tau^3+44\tau^4)\\&\quad \text{for } l=3.\end{aligned} \tag{24}$$

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

$$V(x)=V_0+ax^2-bx^4+cx^6, \tag{25}$$

with $a,b,c>0$. The potentials occurrring for $l=0$, 1, 2, and 3 are of the form

$$V(x)=V_0+ax^2+bx^4+cx^6+dx^8, \tag{26}$$

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

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

$$V_{SWS}(r)=-V_0\frac{\sinh(R/a)}{\cosh(r/a)+\cosh(R/a)},\quad 0\leqslant r\leqslant\infty, \tag{27}$$

and the wine bottle symmetrized Woods-Saxon potential

$$V_{WB}(r)=-V_0\left(1+\frac{wr^2}{R^2}\right)\frac{\sinh(R/a)}{\cosh(r/a)+\cosh(R/a)},\quad 0\leqslant r\leqslant\infty, \tag{28}$$

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

$$\frac{V_{SWS}(r)}{V_0\sinh(R/a)}=-\frac{1}{1+\cosh(R/a)}+\frac{1}{2(1+\cosh(R/a))^2}\frac{r^2}{a^2}-\frac{5-\cosh(R/a)}{24(1+\cosh(R/a))^3}\frac{r^4}{a^4}+\frac{(\cosh(R/a))^2-28\cosh(R/a)+61}{720(1+\cosh(R/a))^4}\frac{r^6}{a^6}, \tag{29}$$

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

The following comments can now be made.

(i) The Taylor expansions of the symmetrized Woods-Saxon and wine bottle symmetrized Woods-Saxon potential, 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 three-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 three-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 three-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 obtains an exponential form. For example, Eq. (10) becomes (for $\tau>0$)

$$E_q(n,n)=\hbar\omega_0\frac{e^{2\tau n}-e^{-2\tau n}}{e^{2\tau}-e^{-2\tau}}\simeq\hbar\omega_0\frac{e^{2\tau n}}{e^{2\tau}-e^{-2\tau}}. \tag{31}$$

Potentials with exponential spectra were considered in Ref. [47], but 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 was found to describe reasonably well the magic numbers of alkali clusters [6]) were determined in Ref. [38]. They have the forms

$$U_3(r)=-\frac{2v}{R^4}\frac{(r/R)^4}{[(r/R)^6+1]^2}, \tag{32}$$

$$V_{\tilde{3}}(r)=E-\frac{2L_m^2}{mR_m^2}\frac{(r/R_m)^4}{[(r/R_m)^6+1]^2}. \tag{33}$$

Both of them are of the form

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

which corresponds to a Taylor expansion of the form

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

We remark that this Taylor expansion bears no similarity to the Taylor expansions of the symmetrized Woods-Saxon potential and wine bottle symmetrized Woods-Saxon potential, 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 a strongly exaggerated wine bottle feature [38], lacking in parallel the flat bottom characterizing the Woods-Saxon and Ekardt potentials. However potential $U_3(r)$ has the major advantage that it reproduces the edge behavior of the Ekardt potentials quite well [38].

VIII. DISCUSSION

The following general remarks can now be made.

(i) From the results reported above it is quite clear that the three-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 value ($\tau=0.020$). 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 three-dimensional q-deformed harmonic oscillator reproduces long sequences of magic numbers (Na, Cs, Li, and Ag) at least as accurately as other, more sophisticated, models by using only one free parameter ($q=e^{\tau}$). (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 δ being the only exception. However, the choice of the value of the energy gap δ does not influence the order of the energy levels, but just decides which energy separations will be considered as corresponding to main magic numbers and which will not. The successful prediction of the magic numbers can be considered as evidence that the three-dimensional q-deformed harmonic oscillator possesses a symmetry [the $\mathrm{u}_q(3)\supset \mathrm{so}_q(3)$ symmetry] appropriate for the description of the physical systems under study.

(iii) As we have already mentioned, it was 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 three-dimensional isotropic harmonic oscillator) characterized by the same $2n+l$ is due to the su(3) symmetry of this system. $3n+l$ was used [6] to approximate the magic numbers of alkali-metal clusters with some success, and focusing potentials characterized by this degeneracy were 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 [$\mathrm{u}_q(3)$], which is a nonlinear extension of the Lie symmetry u(3).

(iv) The ability of the three-dimensional q-deformed harmonic oscillator to reproduce correctly the magic numbers of several metal clusters is not 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 potential and wine bottle symmetrized Woods-Saxon potential, which successfully fit [26,27] the Ekardt potentials [24], which characterize the structure of metal clusters.

In summary, we have shown that the three-dimensional q-deformed harmonic oscillator with $\mathrm{u}_q(3)\supset \mathrm{so}_q(3)$ 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 $\mathrm{u}_q(3)$, which is a nonlinear deformation of the u(3) symmetry of the spherical (three-dimensional isotropic) harmonic oscillator, is a good candidate for the symmetry of systems of several metal clusters. Furthermore, the Taylor expansions of potentials giving approximately the same spectrum as the three-dimensional q-deformed harmonic oscillator are found to have the same form as the Taylor expansions of the symmetrized Woods-Saxon potential and wine bottle symmetrized Woods-Saxon potential, 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. Also an open problem is the existence of any deeper relation between these potentials and the quantum algebra characterizing the three-dimensional q-deformed harmonic oscillator, as, for example, some relation between these potentials and the generators of the quantum algebra.

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