Multidimensional Isotropic and Anisotropic q-Oscillator Models

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Abstract

q-oscillator models are considered in two and higher dimensions and their symmetries are explored. New symmetries are found for both isotropic and anisotropic cases. Applications to the spectra of triatomic molecules and superdeformed nuclei are discussed.

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1 Introduction

The q-deformed oscillator introduced recently [1] has spurred a great deal of activity. Various aspects of the standard harmonic oscillator have been generalized to the q-deformed case [2]. In addition to studies on models with a single q-oscillator and its successful application to different branches of physics [3-8], higher-dimensional isotropic and anisotropic q-oscillator models too have begun to be studied [9-11].

It is known that the generalization of harmonic oscillator to q-oscillator models becomes a nontrivial problem in higher dimensions, even in the isotropic case. In [9] two such two-dimensional isotropic q-oscillator models were proposed. However, only one of them was really analysed, a more natural candidate being ignored. One of our aims is to reconsider this important issue and show that this alternative model also exhibits an interesting symmetry. Our main purpose however is to concentrate on the symmetries of the anisotropic q-oscillator models in two and higher dimensions, which to our knowledge have not been explored properly. It should be emphasized here that the symmetries of the standard (q=1) anisotropic oscillators in two dimensions are well understood [12].

We derive our basic results first for $SU_q(N)$ with $N = 2$ and subsequently extend them to higher $N$. We find interesting applications of our results to the vibrational spectra of triatomic molecules as well as to the shell structure of superdeformed nuclei.

The plan of the paper is as follows. In Section 2 we review ordinary oscillators, both isotropic and anisotropic, so that it will be easier to make the transition to q-oscillators. In Section 3, we discuss isotropic q-oscillators and in Section 4, anisotropic q-oscillators. These two dimensional studies are extended to three dimensions in Section 5. Section 6 discusses some applications.

2 Symmetries of standard oscillators

Let us begin by briefly discussing the ordinary isotropic oscillator model in two dimensions. The Hamiltonian is given by

$$h = \sum_{i=1}^{2} \{a_i^\dagger, a_i\} = (n_1 + n_2 + 1), \quad (1)$$

where $n_i = a_i^\dagger a_i$ is the number operator and $a_i^\dagger, a_i \ (i = 1, 2)$ are ladder operators with commutation relations

$$[a_i, a_j^\dagger] = \delta_{ij}, \ [a_i, a_j] = 0, \ [n_i, a_i] = -a_i. \quad (2)$$

"Angular momentum operators" may be constructed by the Schwinger representation

$$j_+ = a_1^\dagger a_2, \quad j_- = a_2^\dagger a_1, \quad j_3 = \frac{1}{2}(n_1 - n_2). \quad (3)$$

They satisfy the $SU(2)$ algebra and commute with the Hamiltonian which is related to the Casimir operator:

$$j_\alpha j_\alpha = \frac{1}{4}(h^2 - 1).$$
This gives the $SU(2)$ symmetry of the Hamiltonian (1).

Now we ask what happens when the ordinary oscillator model (1) is made anisotropic giving the Hamiltonian
\[ H \propto \omega_1 (n_1 + \frac{1}{2}) + \omega_2 (n_2 + \frac{1}{2}). \]
Of course there is no degeneracy in general, but the spectrum becomes interesting when the frequencies $\omega_1, \omega_2$ are rational multiples of each other. The Hamiltonian is then written as
\[ H = \frac{1}{k_1} (n_1 + 1) + \frac{1}{k_2} (n_2 + 1). \]
with $\omega_1 : \omega_2 = k_1^{-1} : k_2^{-1}$, where $k_1$ and $k_2$ are relatively prime integers. This simple situation has been discussed in the literature [12]. In this anisotropic case in two dimensions an $SU(2)$ symmetry is involved again, though with a curious multiplicity $k_1k_2$ of copies of each irreducible representation of the corresponding algebra. To explain the basic idea behind such symmetries we first note that the reason why the operators $j_\pm$ commute with the Hamiltonian $h$ (1) is that they shift both $n_1, n_2$ by unity but in opposite ways:
\[ f(n_1, n_2)j_\pm = j_\pm f(n_1 \pm 1, n_2 \mp 1). \]
When we go on to the anisotropic Hamiltonian (4) we need ”angular momentum operators” which shift $n_1, n_2$ by different amounts:
\[ f(n_1, n_2)J_\pm = J_\pm f(n_1 \pm k_1, n_2 \mp k_2). \]
Note that the single-quantum shift operator $e^{i\phi}$ which may be associated with the standard creation operator through $a^\dagger = \sqrt{n}e^{i\phi}$ shifts $n$ by unity: $f(n)e^{i\phi} = e^{i\phi}f(n + 1)$. We construct in analogy a multi-quantum shift operator $e^{ik\phi}$ and a corresponding multi-quantum creation operator $A^\dagger = \sqrt{N}e^{ik\phi}$, where $N = \left[\frac{n}{k}\right]$, the integral part of $\frac{n}{k}$, i.e.,
\[ n = Nk + r, \quad (0 \leq r < k). \]
The operators $A, A^\dagger$ thus constructed, together with their number operator $N$, satisfy the usual oscillator algebra:
\[ [A_i, A_j^\dagger] = \delta_{ij}, [A_i, A_j] = 0, [N, A_i] = -A_i. \]
Writing out the shift operators $e^{ik\phi} = (n^{-\frac{1}{2}}a^\dagger)^k$, one finally arrives at
\[ A^\dagger = \sqrt{N} \left( \frac{(n-k)!}{n!} \right)^{\frac{1}{2}} a^\dagger. \]
Note that these creation and annihilation operators depend on both $N$ and $r$ apart from the usual creation and annihilation operators, but the number operator $N$ is independent of $r$. These bosonic operators are the same as the generalized bosons introduced earlier in other contexts [12]. With their help one may easily construct ”angular momentum operators” [12] for the anisotropic case by direct analogy with the isotropic one:
\[ J_+ = A_1^\dagger A_2, \quad J_- = A_2^\dagger A_1, \quad J_3 = \frac{1}{2}(N_1 - N_2), \]
where the appropriate \( k_i \) are understood to be used in the construction of \( A_i \) from \( a_i \) \((i = 1, 2)\). It may be noted that unlike \( J_\pm \), which depend on both \( N \) and \( r \) apart from the operators \( a, a^\dagger, J_3 \) depends only on \( N \).

Due to the validity of the bosonic commutation relations (6), the generators (8) provide again a Schwinger type realization of \( SU(2) \) and because of the modified shifts, they commute with the Hamiltonian (4).

The usual \( SU(2) \) quantum numbers are given by \( J = \frac{1}{2}(N_1 + N_2), M = \frac{1}{2}(N_1 - N_2) \) and the energy can be written as

\[
E(J, r_1, r_2) = 2J + \frac{r_1 + \frac{1}{2}}{k_1} + \frac{r_2 + \frac{1}{2}}{k_2}.
\]

Thus the remainders \( r_1, r_2 \) enter the expression for the energy here, which is not completely determined by \( J \). These remainders can take \( k_1 \) and \( k_2 \) different values respectively. Note that if \( J, M, r_1 \) and \( r_2 \) are all specified then \( n_1, n_2 \) and hence the states are fixed. Now for given values of \( r_1, r_2 \), the \( SU(2) \) quantum numbers \( J, M \) can vary as usual and every irreducible representation of the group occurs exactly once. By varying \( r_1, r_2 \), one therefore obtains \( k_1k_2 \) copies of each irreducible representation of \( SU(2) \). These \( k_1k_2 \) copies all have different energy, as is clear from (9) above. Note that for \( k_1 = k_2 = 1 \) we recover the isotropic case with only one copy of each irreducible representation. Higher dimensional generalizations can be made by exploiting these ideas of two dimensions and lead to an \( SU(N) \) symmetry. One interesting possibility should be noted here. If we regard the different levels for a fixed value of \( j \) as forming a bunch, the spread of energy values within a bunch may be so large that the bunches overlap violating the level sequence. Whereas in the isotropic case levels with higher values of \( j \) have necessarily higher energies than levels with lower \( j \), in the anisotropic case, \( E(J, r_1, r_2) \) exceeds \( E(J + \frac{1}{2}, r'_1, r'_2) \) if

\[
\frac{(r_1 - r'_1)}{k_1} + \frac{(r_2 - r'_2)}{k_2} > 1.
\]

This crossing of levels may be of interest in practical situations.

### 3 Isotropic q-oscillator models

A q-oscillator involves the q-commutators [1]

\[
a^q a^{q\dagger} - q a^q a^{q\dagger} = q^{-n}, \quad [n, a^q] = -a^q,
\]

where we take \( q = e^{i\alpha} \) not to be a root of unity. One can use two independent sets of such operators to construct generators

\[
j^q_+ = a^q a^{q\dagger}_2, j^q_- = a^{q\dagger}_2 a^q, j^q_3 = \frac{1}{2} (n_1 - n_2)
\]

satisfying the \( SU_q(2) \) algebra [1]

\[
[j^q_+, j^q_-] = [2j^q_3]q, \quad [j^q_3, j^q_3] = \pm j^q_3.
\]
Here $[x]_q$ stands for \( \frac{x^q - q^{-x}}{q - q^{-1}} = \frac{\sin q x}{\sin \alpha} \).

A candidate [9] for the isotropic q-oscillator Hamiltonian is (1) itself or its q-deformation:

\[
h_i^q = [n_1 + n_2 + 1]_q
\]

(10)

All the generators of the $SU_q(2)$ algebra introduced above commute with the Hamiltonian (10) and in fact with an arbitrary function of $n_1 + n_2 + 1$. Thus, (1) itself, (10), or an arbitrary function of $n_1 + n_2 + 1$ and $q$, which reduces to (1) when $q$ goes to unity, can be taken as the Hamiltonian for the isotropic q-oscillator. We shall refer to such Hamiltonians as being of Type I. Note that only the undeformed expression (or a linear function thereof) can be expressed as a sum of two similar terms for the two individual oscillators. An interesting property of such systems is that there are violations of the level sequence. This is due to the fact that an inequality $n' > n$ cannot guarantee the inequality $[n']_q > [n]_q$, which holds only for small values of $n, n'$ and $\alpha$. For such values, the energy spectrum is similar to the standard case. For higher values of these quantities, however, the energy sequence is violated. The dependence of $[n]_q = \frac{\sin n \alpha}{\sin \alpha}$ on the parameter $\alpha$ also gives a bound $| [n]_q | < | \sin \alpha |^{-1}$, limiting the energy spectrum in a bounded range. Different levels however will not coincide as long as $q$ is not a root of unity.

There is a more natural choice for the Hamiltonian of the isotropic two-dimensional q-oscillator. This is the sum of the Hamiltonians for two independent q-oscillators:

\[
h_{II}^q = \frac{1}{2} \left\{ a_i^q, a_i^q \right\} = [n_1 + \frac{1}{2}]_q + [n_2 + \frac{1}{2}]_q.
\]

(11)

As mentioned above, this model was briefly taken up in [4] where it was pointed out that it does not commute with the generators (3' of the $SU_q(2)$ algebra. We shall refer to it as being of Type II. Note that its spectrum has obvious degeneracies arising from the permutibility of the two q-oscillators. As we have restricted ourselves to the situation where $q$ is not a root of unity, there are in general no multiplets besides doublets (and singlets). It turns out that the permutation symmetry may induce an interesting $SU(2)$ or $SU_q(2)$ symmetry in this spectrum, as can be seen in the following way. The algebra is made up of the operators

\[
\tilde{j}_+ = \sum_{i=0}^{\infty} \sum_{n=1}^{\infty} \frac{[i]_q!}{[i+n]_q!} \langle \tilde{j}_+^q \rangle^n | i, i + n \rangle \langle i, i + n |
\]

\[
= \sum_{i=0}^{\infty} \sum_{n=1}^{\infty} | i + n, i \rangle \langle i, i + n |,
\]

\[
\tilde{j}_- = \tilde{j}_+^\dagger,
\]

\[
\tilde{j}_3 = \frac{1}{2} \sum_{i=0}^{\infty} \sum_{n=1}^{\infty} \left[ | i + n, i \rangle \langle i + n, i | - | i, i + n \rangle \langle i, i + n | \right].
\]

(12)

Each term in the expansion of $\tilde{j}_+$ projects out the state $| i, i + n \rangle$ and in view of the representation (3') and the relations

\[
a_i^q | n_i \rangle = \sqrt{[n]_q} | n_i - 1 \rangle, \quad a_i^{\dagger q} | n_i \rangle = \sqrt{[n + 1]_q} | n_i + 1 \rangle
\]
\((j_+^q)^n\) takes a state with \(n_1 = i, n_2 = i + n\) to a state with \(n_1 = i + n, n_2 = i\) by creating \(n\) quanta of the first kind while destroying an equal number of quanta of the second kind. Similarly terms of \(\tilde{j}_-\) act in the reverse way. These operators satisfy the \(SU(2)\) algebra, which can be checked easily by direct calculation. They even satisfy the \(SU_q(2)\) algebra. This happens because the operator \(\tilde{j}_3\) has only zero and one-half as eigenvalues as a result of the easily verifiable property \((\tilde{j}_+)^2 = (\tilde{j}_-)^2 = 0\), and for these eigenvalues, \(SU(2)\) and \(SU_q(2)\) are identical. It can be checked easily that the above operators commute with (5) and therefore the Hamiltonian can be said to have an \(SU(2)\) or \(SU_q(2)\) symmetry. However, this symmetry manifests itself only in doublets and singlets, in contrast to the infinite variety of representations that is observed for the \(SU(2)\) symmetry of (1) and the \(SU_q(2)\) symmetry of (10).

### 4 Anisotropic q-oscillators

Let us go over to the anisotropic q-oscillator of Type I. The Hamiltonian \(H^q_I\) in the isotropic case obviously commutes with the \(SU_q(2)\) generators introduced above, but an anisotropic Hamiltonian

\[
H^q_I = \frac{1}{k_1}(n_1 + \frac{1}{2}) + \frac{1}{k_2}(n_2 + \frac{1}{2})_q,
\]

(13)

where \(k_1, k_2\) are unequal, positive integers having no common factor, does not do so. However one finds that, much as before, \(q\)-creation and annihilation operators may be introduced through the unit quantum shift operator as \(a^{q\dagger} = \sqrt{[n]_q}e^{iP}\), and through the multi-quanta shift operator as \(A^{q\dagger} = \sqrt{[N]_q}e^{ikP}\) giving

\[
A^{q\dagger} = \sqrt{[N]_q} \left( \frac{[n_i - k]_q}{[n_i]_q!} \right)^{\frac{1}{2}} (a^{q\dagger})^{k_i}.
\]

(14)

Here, \([n]_q = [n]_q[n-1]_q...[1]_q\) and \(N_i\) stands for the integral part already introduced in the standard case. The operators (14) proposed recently [13] as generalized \(q\)-bosons can be used to construct generators

\[
J^q_+ = A^{q\dagger}A^q_2, \quad J^q_- = A^{q\dagger}A^q_1, \quad J^q_3 = \frac{1}{2}(N_1 - N_2)
\]

(15)

satisfying the same \(SU_q(2)\) algebra. It is interesting to note that the generators \(J^q_3\), \(J^q_3\) thus constructed commute with the Hamiltonian \(H^q_I\). Therefore we conclude that anisotropic type I q-oscillator model (13) exhibits again the \(SU_q(2)\) symmetry as done by its isotropic counterpart (10). Moreover, because of the splitting of \(\frac{n}{k}\) into its integral part \(N_i\) and the fractional part \(\frac{r_i}{k}\), exactly as before, there are \(k_1 k_2\) copies of each representation of \(SU_q(2)\). These copies have different energies as long as \(q\) is not a root of unity. Thus, although the nonlinear expression for the energy may change the ordering of the levels from the standard situation, the degeneracies remain exactly the same as before with the expression of energy given by

\[
E^q_I(J, r_1, r_2) = [2J + \frac{r_1 + \frac{1}{2}}{k_1} + \frac{r_2 + \frac{1}{2}}{k_2}]_q.
\]

(9')
Next we come to the case of anisotropic q-oscillators of Type II. The Hamiltonian is taken to be

$$H_{II}^q = \left[ \frac{1}{k_1} (n_1 + \frac{1}{2}) \right]_q + \left[ \frac{1}{k_2} (n_2 + \frac{1}{2}) \right]_q. \quad (16)$$

By separating the integral and fractional parts as before, we can write this as

$$H_{II}^q = \left[ N_1 + \frac{2r_1 + 1}{2k_1} \right]_q + \left[ N_2 + \frac{2r_2 + 1}{2k_2} \right]_q. \quad (17)$$

However contrary to the isotropic case (11) this expression in general does not exhibit the permutation symmetry under exchange of $N_1$ and $N_2$, because of the fractions which are different in the two terms. It is easy to see that these fractions can be equal only when $2r_i + 1 = k_i$ for $i = 1, 2$ i.e., only fixed values of $r_i$ determined by given $k_i$ can lead to degenerate levels. Thus there is a very limited amount of degeneracy in the states of this system and it occurs only if neither $k_i$ is even. When these restrictions on $k_i$ and $r_i$ are satisfied, there occur doublets (and singlets) much as in the isotropic case of Type II. There is again an $SU(2)$ or equivalently $SU_q(2)$ symmetry underlying these multiplets. The corresponding generators can be constructed as in (12) with only the replacement of the generators (3') by the anisotropic ones (15) having the properties

$$A^q_i \ | N_i \rangle = \sqrt{[N_i]_q} \ | N_i - 1 \rangle \ , \ A^{q\dagger}_i \ | N_i \rangle = \sqrt{[N_i + 1]_q} \ | N_i + 1 \rangle.$$ 

Thus in terms of the operators $J^q_+, J^q_3$, introduced for the anisotropic q-oscillator of Type I and appropriate projection operators, we may write

$$\tilde{J}^q_+ = \sum_{I=0}^{\infty} \sum_{N=1}^{\infty} \frac{[I]_q!}{[I + N]_q!} (J^q_+)^N \ | I, I + N; r_1, r_2 \rangle \langle I, I + N; r_1, r_2 |$$

$$= \sum_{I=0}^{\infty} \sum_{N=1}^{\infty} | I + N, I; r_1, r_2 \rangle \langle I + N, I; r_1, r_2 |,$$

$$\tilde{J}^q_3 = \frac{1}{2} \sum_{I=0}^{\infty} \sum_{N=1}^{\infty} \left[ | I + N, I; r_1, r_2 \rangle \langle I + N, I; r_1, r_2 | - | I, I + N; r_1, r_2 \rangle \langle I, I + N; r_1, r_2 | \right]. \quad (18)$$

Here the states are understood to be labelled by their quantum numbers $N_1$, $N_2$, $r_1$, $r_2$ with fixed values $r_i = \frac{k_i - 1}{2}$. Repeating similar arguments it may be shown that the operators introduced in (18) not only obey the $SU(2)$ or $SU_q(2)$ algebra but also commute with the Hamiltonian (16) and thus can be said to be responsible for the degeneracy of the states. As in the case of the corresponding isotropic q-oscillator, only the spin one-half (and zero) representations occur instead of the infinite variety observed for Type I.

5 Higher dimensional models

After this elaborate discussion of two dimensional oscillators, its generalization to higher dimensions does not pose any difficulty. For example, while the ordinary isotropic three dimensional oscillator with the Hamiltonian $H = n_1 + n_2 + n_3$ exhibits an $SU(3)$ symmetry
with certain irreducible representations (the symmetric tensor ones) occurring exactly once, the anisotropic Hamiltonian \( \tilde{H} = \frac{n_1}{k_1} + \frac{n_2}{k_2} + \frac{n_3}{k_3} \) leads to an \( SU(3) \) with each of the above representations occurring \( k_1 k_2 k_3 \) times, the integers \( k_i \) being assumed to contain no overall common factor. Just as the generators of the algebra in the isotropic case can be written as \( a_1^{\dagger}a_2, a_2^{\dagger}a_3, a_1^{\dagger}a_3 \), their conjugates and the elements of the Cartan subalgebra \( \frac{1}{2}(n_1 - n_2), \frac{1}{2}(n_2 - n_3) \), in the anisotropic case one replaces \( a_i, n_i \) by \( A_i, N_i \) defined with the appropriate \( k_i \) involved in the Hamiltonian. Repetition of multiplets occurs because the energy contains a new piece \( \frac{r_1}{k_1} + \frac{r_2}{k_2} + \frac{r_3}{k_3} \), where \( r_i \) varies from 0 to \( k_i - 1 \).

Apart from the possibility of overlapping bunches already seen in the case of two dimensions, a new peculiarity may appear here. As there are several \( k_i \)s, it may so happen that although there is no overall common factor between them, some of them possess some common factor. In that case, there will exist different multiplets with equal energies. For instance, if \( k_1 = 4, k_2 = 2, k_3 = 1 \), the copies of any multiplet with \( r_1 = 2, r_2 = 0 \) and \( r_1 = 0, r_2 = 1 \) will have equal energies. Thus the symmetry generators do not connect all states having the same energy.

More generally, in the \( \nu \) dimensional case, the anisotropic Hamiltonian \( \tilde{H} = \sum_{i=1}^{\nu} \frac{n_i}{k_i} \) leads to \( \prod_1^{\nu} k_i \) copies of each irreducible representation of \( SU(N) \) observed in the isotropic case. It is assumed here that the \( k_i \)s are integers containing no overall common factor. The peculiarities occurring in the lower dimensional cases can of course occur here as well.

Similarly such higher dimensional cases can be considered with q-deformations leading to an \( SU_q(N) \) symmetry in both the isotropic and anisotropic cases. The construction of symmetry operators in the anisotropic case is analogous to the undeformed situation; as in the two dimensional case, the bosonic operators should be replaced by their q-deformations.

For the three dimensional q-oscillator of Type II one may take the generators as

\[
\tilde{j}_{12} = \sum_{i=0}^{\infty} \sum_{n=1}^{\infty} \sum_{n_3=0}^{\infty} |i + n, i, n_3 \rangle \langle i, i + n, n_3 |,
\]

\[
\tilde{j}_{13} = \sum_{i=0}^{\infty} \sum_{n=1}^{\infty} \sum_{n_2=0}^{\infty} |i + n, n_2, i \rangle \langle i, n_2, i + n |,
\]

\[
\tilde{j}_3 = \frac{1}{2} \sum_{i=0}^{\infty} \sum_{n=1}^{\infty} \sum_{n_3=0}^{\infty} [ |i + n, i, n_3 \rangle \langle i + n, i, n_3 | - |i, i + n, n_3 \rangle \langle i, i + n, n_3 | ],
\]

(19)

etc with the property \( \tilde{j}_{ij}^2 = 0 \).

6 Some physical applications

The three dimensional generalization of the Type I model has interesting physical applications. The Hamiltonian in this case is

\[
H_I^q = \left[ \frac{1}{k_1} (n_1 + \frac{1}{2}) + \frac{1}{k_2} (n_2 + \frac{1}{2}) + \frac{1}{k_3} (n_3 + \frac{1}{2}) \right]_q.
\]

(20)
The generalized $SU_q(3)$ generators are given by
\[ J_{12}^q = A_1^q A_2^q, \quad J_{13}^q = A_1^q A_3^q, \quad J_3^q = \frac{1}{2}(N_1 - N_2), \] (21)
etc. The Hamiltonian exhibits $SU_q(3)$ symmetry with a spectrum containing $k_1k_2k_3$ copies of each symmetric tensor representation of $SU_q(3)$. Considering $\alpha$ to be small, we expand (20) as
\[ H_q^I \approx (1 + \frac{\alpha^2}{3!})H - \frac{\alpha^2}{3!}H^3, \] (22)
where $H$, the $q=1$ part of (20), is given by
\[ \omega H = \omega_1(n_1 + \frac{1}{2}) + \omega_2(n_2 + \frac{1}{2}) + \omega_3(n_3 + \frac{1}{2}) \] (23)
with zero-order frequencies $\omega_i$ corresponding to its normal modes. We find that there exists an interesting connection between our model and the spectra of triatomic molecules as well as superdeformed nuclei. Though there exist a number of investigations showing the agreement of q-oscillator models with the experimentally observed vibrational and rotational spectra of some diatomic molecules with surprising accuracy [5,6], similar studies on triatomic molecules are scarce, and even when available, are restricted to the isotropic case [10]. On the other hand, the Hamiltonian (20) and hence (22) for small $q$-values can possibly be applied to explain vibrational spectra of a class of real triatomic molecules with the inclusion of anharmonicity along with the anisotropy given in rational ratios. That is, for triatomic molecules with normal modes in the ratios
\[ \omega_1 : \omega_2 : \omega_3 = \epsilon_1 n_1 : \epsilon_2 n_2 : \epsilon_3 n_3, \]
where the $n_i$-s are integers while $\epsilon_i$-s are numbers close to unity showing deviations from rational ratios. For example, our model is expected to describe the vibrational spectra of molecules like [15]

1. HOCl, with zero-order frequencies (in cm$^{-1}$)
\[ \omega_1 = 3609, \quad \omega_2 = 1238, \quad \omega_3 = 720, \] (24a)
in the ratio $\omega_1 : \omega_2 : \omega_3 \approx 5 : 2 : 1$ with accuracy
\[ \epsilon_1 = 1.00, \quad \epsilon_2 = 0.86, \quad \epsilon_3 = 1.00. \] (24b)

2. HDO, with zero-order frequencies (in cm$^{-1}$)
\[ \omega_1 = 2724, \quad \omega_2 = 1403, \quad \omega_3 = 3707, \] (25a)
in the ratio $\omega_1 : \omega_2 : \omega_3 \approx 2 : 1 : 3$ with accuracy
\[ \epsilon_1 = 0.97, \quad \epsilon_2 = 1.00, \quad \epsilon_3 = 0.88. \] (25b)
3. $\text{H}_2\text{O}$, with zero-order frequencies (in cm$^{-1}$)

$$\omega_1 = 3825.3, \quad \omega_2 = 1653.9, \quad \omega_3 = 3935$$

in the ratio $\omega_1 : \omega_2 : \omega_3 \approx 2 : 1 : 2$ with accuracy

$$\epsilon_1 = 1.16, \quad \epsilon_2 = 1.00, \quad \epsilon_3 = 1.19.$$  \hfill (26b)

For demonstrating our claim, we present here in detail the case of the water molecule. The vibrational spectra of $\text{H}_2\text{O}$ molecules (without considering the anharmonicity) may be described by the Hamiltonian (23) [14,15] rewritten as

$$\omega H = \omega \left( \epsilon_1 (n_1 + \frac{1}{2}) + \frac{\epsilon_2}{2} (n_2 + \frac{1}{2}) + \epsilon_3 (n_3 + \frac{1}{2}) \right)$$

with $\omega = 3307.8$ and $\epsilon_i$ as given in (26b). We see that our anisotropic model (20) for $k_1 : k_2 : k_3 = 1 : 2 : 1$ and $q = 1$ can describe this system with fairly good accuracy. The system thus has an approximate $SU(3)$ symmetry when anharmonic effects are neglected.

For describing the experimental result more accurately anharmonic terms are usually considered and for triatomic molecules like $\text{H}_2\text{O}$ the number of such anharmonic parameters is six. We show in Table 1 that our single-parameter $q$-oscillator model can also describe such anharmonic effects with good accuracy. The energy spectrum obtained from our formula (22) including anharmonicity is shown in the penultimate column of Table 1. Note its close resemblance with the spectrum of $\text{H}_2\text{O}$ given in the last column, which is calculated from the 6-parameter fit of [15]. Here $E(\text{anh}-q)$ is a single parameter fit, where $\alpha=0.0849$ is chosen to get the best fit with the 6-parameter result within the given range.

This suggests that the vibrational Hamiltonian of $\text{H}_2\text{O}$ molecules with anharmonicity exhibits an approximate $SU_q(3)$ symmetry (with $q = \exp(0.0849)$) along with all the interesting features of the anisotropic $q$-oscillator model discussed here.

As another possible application, one should mention that in analysing the shell structure of superdeformed nuclei one usually considers the energy spectrum [16]

$$E(n_1, n_2, n_3) = \hbar \omega_\perp (n_1 + n_2 + 1) + \hbar \omega_3 (n_3 + \frac{1}{2})$$

The major shell structure is observed only when $\omega_\perp$ and $\omega_3$ are in the ratios of small integers. The reason behind this fact and the symmetry involved are not well understood, as stressed by Mottelson [16]. We see here that such superdeformed nuclear models with nonlinear terms may well be represented by our anisotropic $q$-oscillator with an $SU_q(3)$ symmetry, which may be a preferred symmetry providing a stable structure.

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Table 1: Energy spectrum $E = \omega H^q_1$, where $H^q_1$ is as in (22) with $\alpha = 0.0849$. $E(\text{anh} - q)$ and $E_0$ give the values with and without consideration of the anharmonicity, while $E(\text{exp})$ was obtained from [15].

| $n1$ | $n2$ | $n3$ | $E0$  | $E(\text{anh-q})$ | $E(\text{exp})$ |
|------|------|------|-------|------------------|-----------------|
| 0    | 0    | 0    | 4707  | 4701             | 4680            |
| 0    | 1    | 0    | 6361  | 6340             | 6295            |
| 0    | 2    | 0    | 8015  | 7968             | 7871            |
| 1    | 0    | 0    | 8531  | 8473             | 8419            |
| 0    | 0    | 1    | 8643  | 8583             | 8524            |
| 0    | 3    | 0    | 9669  | 9581             | 9408            |
| 1    | 1    | 0    | 10185 | 10081            | 10102           |
| 0    | 1    | 1    | 10297 | 10190            | 10121           |
| 0    | 4    | 0    | 11323 | 11177            | 10906           |
| 1    | 2    | 0    | 11839 | 11671            | 11746           |
| 0    | 2    | 1    | 11951 | 11778            | 11678           |
| 2    | 0    | 0    | 12355 | 12162            | 12075           |
| 1    | 0    | 1    | 12467 | 12269            | 12107           |
| 0    | 0    | 2    | 12580 | 12376            | 12277           |
| 0    | 5    | 0    | 12977 | 12752            | 12365           |
| 1    | 3    | 0    | 13493 | 13239            | 13351           |
| 0    | 3    | 1    | 13605 | 13345            | 13197           |
| 2    | 1    | 0    | 14009 | 13724            | 13825           |
| 1    | 1    | 1    | 14121 | 13829            | 13771           |
| 0    | 1    | 2    | 14233 | 13934            | 13855           |
| 1    | 4    | 0    | 15146 | 14783            | 14917           |
| 0    | 4    | 1    | 15259 | 14887            | 14676           |
| 2    | 2    | 0    | 15662 | 15259            | 15537           |
| 1    | 2    | 1    | 15775 | 15363            | 15396           |
| 0    | 2    | 2    | 15887 | 15466            | 15393           |
| 3    | 0    | 0    | 16178 | 15733            | 15645           |
| 2    | 0    | 1    | 16291 | 15836            | 15605           |
| 1    | 0    | 2    | 16403 | 15938            | 15702           |
| 0    | 0    | 3    | 16516 | 16041            | 15937           |
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