Coupled Q-oscillators as a model for vibrations of polyatomic molecules

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Abstract

The system of two Q-deformed oscillators coupled so that the total Hamiltonian has the su_Q(2) symmetry is proved to be equivalent, to lowest order approximation, to a system of two identical Morse oscillators coupled by the cross-anharmonicity usually used empirically in describing vibrational spectra of triatomic molecules. The symmetry also imposes a connection between the self-anharmonicity of the Morse oscillators and the cross-anharmonicity strength, which can be removed by replacing the Q-oscillators by deformed anharmonic oscillators. The generalization to n oscillators is straightforward. The applicability of the formalism to highly symmetric polyatomic molecules is discussed.

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Quantum algebras (also called quantum groups)\textsuperscript{1,2}, are recently receiving much attention in physics. They are $q$-deformations of the universal enveloping algebras of the corresponding Lie algebras, to which they reduce when the deformation parameter $q$ is set equal to 1. From the mathematical point of view they are Hopf algebras\textsuperscript{3}. Initially used for solving the quantum Yang Baxter equation\textsuperscript{4}, they are now finding applications in several branches of physics, especially after the introduction of the $q$-deformed harmonic oscillator\textsuperscript{5–7}. Applications in conformal field theory, quantum gravity, quantum optics, atomic physics, nuclear physics, as well as in the description of spin chains have already appeared.

In molecular physics rotational spectra of diatomic molecules have been described in terms of the $su_q(2)$ symmetry\textsuperscript{8,9}. For vibrational spectra of diatomic molecules both $q$-deformed harmonic\textsuperscript{10} and $q$-deformed anharmonic\textsuperscript{11} oscillators have been successfully used and WKB equivalent potentials giving the same spectrum as these oscillators have been determined\textsuperscript{12}, related to a $q$-deformation of the modified Pöschl Teller potential, which is connected to the Morse potential by a known transformation\textsuperscript{13}. A review of applications of quantum algebraic techniques in diatomic molecules has been given in\textsuperscript{14}.

The success of the quantum algebraic description in vibrational spectra of diatomic molecules creates the question if an extension to vibrational spectra of triatomic and polyatomic molecules is possible. Vibrational spectra of triatomic and polyatomic molecules have been traditionally described in terms of coupled oscillators\textsuperscript{15–19}. Recently, a model of coupled anharmonic oscillators, in which each bond in a polyatomic molecule is replaced by a Morse potential, has also appeared\textsuperscript{20–23}. (This model is a simplification of the vibron model\textsuperscript{24,25}, in which both rotations and vibrations are treated simultaneously.) On the other hand, the way of coupling $n$ $q$-deformed oscillators so that the total Hamiltonian is characterized by an $su_q(n)$ symmetry has been understood\textsuperscript{26–28}. The spectrum of this system exhibits cross-anharmonicities among the levels of the individual oscillators, imposed by the quantum symmetry. It is therefore worth examining if the cross-anharmonicities imposed by the overall quantum symmetry bear any
similarity to the cross-anharmonicities long used in molecular physics on an empirical basis.

The Hamiltonian usually used for the description of vibrational modes of polyatomic molecules is

\[ H = \sum_i \omega_i \left( v_i + \frac{d_i}{2} \right) + \sum_i \sum_{k \geq i} x_{ik} \left( v_i + \frac{d_i}{2} \right) \left( u_k + \frac{d_k}{2} \right), \]

(1)

where \( v_i, v_k \) are vibrational quantum numbers and \( d_i, d_k \) the degeneracies of the corresponding modes. More specifically, for ABA triatomics a frequently used Hamiltonian reads

\[ H = \hbar \omega_1 \left( n_1 + \frac{1}{2} \right) + \hbar \omega_2 \left( n_2 + \frac{1}{2} \right) \]

\[ + \frac{\gamma_1}{2} \left( n_1 + \frac{1}{2} \right)^2 + \frac{\gamma_2}{2} \left( n_2 + \frac{1}{2} \right)^2 + \gamma_{12} \left( n_1 + \frac{1}{2} \right) \left( n_2 + \frac{1}{2} \right). \]

(2)

It is clear that the first and third term in this Hamiltonian describe an anharmonic oscillator, the second and fourth term describe another anharmonic oscillator, while the fifth term describes the cross-anharmonicity between them. It is worth recalling at this point that the spectrum of the anharmonic oscillators encountered here is the same as the spectrum obtained from solving the Schrödinger equation for the Morse potential.

In recent work \( q \)-numbers are defined as

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

(3)

where \( q \) can be real (\( q = e^\tau \), where \( \tau \) real) or a phase factor (\( q = e^{i\tau} \), with \( \tau \) real). The \( q \)-deformed harmonic oscillator is defined in terms of the creation and annihilation operators \( a^\dagger \) and \( a \) and the number operator \( N \), which satisfy the commutation relations

\[ [N, a^\dagger] = a^\dagger, \quad [N, a] = -a, \quad aa^\dagger - q^\tau a^\dagger a = q^{\pm N}. \]

(4)

The Hamiltonian of the \( q \)-deformed harmonic oscillator is

\[ H = \frac{\hbar \omega}{2} (aa^\dagger + a^\dagger a), \]

(5)

and its eigenvalues are

\[ E(n) = \frac{\hbar \omega}{2} ([n]_q + [n + 1]_q). \]

(6)
Coupling two of these oscillators with the requirement that the total Hamiltonian has the \( \text{su}_q(2) \) symmetry one finds
\[
H = a_1^\dagger a_1 q^{N_2} + q^{-N_1} a_2^\dagger a_2,
\]
the generators of \( \text{su}_q(2) \) in terms of two mutually commuting sets of \( q \)-boson operators \((a_1, a_1^\dagger, N_1)\) and \((a_2, a_2^\dagger, N_2)\) in the Schwinger realization being
\[
J_0 = \frac{1}{2}(N_1 - N_2), \quad J_+ = a_1^\dagger a_2, \quad J_− = a_2^\dagger a_1,
\]
and satisfying the commutation relations
\[
[J_0, J_±] = ±J_±, \quad [J_+, J_-] = [2J_0]_q.
\]
The relevant eigenvalues of the Hamiltonian of Eq. (7) are
\[
E(n_1, n_2) = [n_1 + n_2]_q.
\]
For \( l \) q-deformed harmonic oscillators coupled so that the overall symmetry is \( \text{su}(l) \) one obtains the eigenvalues
\[
E(n_1, n_2, \ldots, n_l) = [n_1 + n_2 + \ldots + n_l]_q.
\]
Using the Taylor expansion
\[
[N]_q = N \pm \frac{\tau^2}{6} (N - N^3) + \frac{\tau^4}{360} (7N - 10N^3 + 3N^5) \pm \cdots,
\]
where the upper (lower) sign corresponds to \( q \) being a phase factor (real), the energy eigenvalues of Eq. (10), including terms up to \( \tau^2 \), can be written as
\[
E(n_1, n_2) = n_1 \left( 1 \pm \frac{\tau^2}{6} \right) \pm \frac{\tau^2}{6} n_1^3 + n_2 \left( 1 \pm \frac{\tau^2}{6} \right) \pm \frac{\tau^2}{6} n_2^3
\]
\[
\mp \frac{\tau^2}{2} (n_1^2 n_2 + n_2^2 n_1) + \ldots
\]
In comparison to the empirical Hamiltonians of Eqs (1) and (2) we remark that:
\[\text{i) The lowest order self-anharmonicities of the oscillators involved in Eq. (13) are proportional to } n_i^3 \text{ and not to } n_i^2 \text{ as in Eqs (1), (2).}\]
ii) The lowest order cross-anharmonicities in Eq. (13) are of the type \( n_i^2 n_j \) and \( n_j^2 n_i \), and not of the type \( n_i n_j \) as in Eqs (1), (2).

iii) The previous two remarks also hold in the case of \( n \) coupled \( q \)-deformed oscillators.

We therefore conclude that the usual coupled \( q \)-deformed oscillators are not suitable for the description of vibrational spectra of polyatomic molecules.

However, a different version of deformed oscillator, the \( Q \)-oscillator \(^{30-32}\), can be simply obtained by defining \(^{32,33}\) the operators \( b, b^\dagger \) through the equations

\[
a = q^{1/2} b q^{-N/2}, \quad a^\dagger = q^{1/2} q^{-N/2} b^\dagger.
\] (14)

Eq. (4) then gives

\[
[N, b^\dagger] = b^\dagger, \quad [N, b] = -b, \quad b b^\dagger - q^2 b^\dagger b = 1.
\] (15)

By using the symbol \( Q = q^2 \) and introducing the \( Q \)-number

\[
[x]_Q = \frac{Q^x - 1}{Q - 1},
\] (16)

where \( Q = e^T \) (with \( T \) real), we have that

\[
b b^\dagger = [N]_Q, \quad b b^\dagger = [N + 1]_Q.
\] (17)

The basis is defined by

\[
b |0> = 0, \quad |n> = \frac{(b^\dagger)^n}{\sqrt{n!}_Q} |0>.
\] (18)

where the \( Q \)-factorial is defined by

\[
[n]_Q! = [n]_Q [n-1]_Q \ldots [2]_Q [1]_Q.
\] (19)

The action of the operators on the basis is given by

\[
N |n> = n |n>, \quad b^\dagger |n> = \sqrt{[n+1]_Q} |n+1>, \quad b |n> = \sqrt{[n]_Q} |n-1>.
\] (20)

The Hamiltonian of the corresponding deformed harmonic oscillator has the form

\[
H = \frac{\hbar \omega}{2} (b b^\dagger + b^\dagger b),
\] (21)
the eigenvalues of which are
\[ E(n) = \frac{\hbar \omega}{2}([n]_Q + [n + 1]_Q). \] (22)

Our next task is to consider a system of two Q-oscillators and construct a Hamiltonian having the su\(_Q(2)\) symmetry. Using two mutually commuting sets of Q-boson operators \((b_1, b_1^\dagger, N_1)\) and \((b_2, b_2^\dagger, N_2)\) one can construct a Schwinger realization of the su\(_Q(2)\) generators, which satisfy the commutation relations

\[ [J_0, J_\pm] = \pm J_\pm, \quad J_+J_- - Q^{-1}J_-J_+ = [2J_0]_Q, \] (23)

in the form

\[ J_0 = \frac{1}{2}(N_1 - N_2), \quad J_+ = (J_-)^\dagger = b_1^\dagger Q^{-N_2/2}b_2. \] (24)

The Casimir operator is

\[ C = Q^{-J_0}([J_0]_Q[J_0 + 1]_Q + Q^{-1}J_-J_+) = Q^{-J_0}(J_+J_- + Q[J_0]_Q[J_0 - 1]_Q). \] (25)

This can be written in the form

\[ C = -\left[ \frac{N_1 + N_2}{2} + 1 \right]_Q \left[ -\frac{N_1 + N_2}{2} \right]_Q, \] (26)

i.e. it depends only on \(N_1 + N_2\). One can easily verify that a Hamiltonian of the form

\[ H = [N_1 + N_2]_Q, \] (27)

commutes with the generators of su\(_Q(2)\) given in Eq. (24), i.e. has the su\(_Q(2)\) symmetry. In order to see the analogy with Eq. (7) one can write Eq. (27) in the form

\[ H = b_1^\dagger b_1 \frac{Q^{N_2} + 1}{2} + \frac{Q^{N_1} + 1}{2} b_2^\dagger b_2. \] (28)

In order to check the physical content of the coupled Q-oscillators of Eq. (27), we use the Taylor expansion

\[ [N]_Q = N + \frac{T}{2}(N^2 - N) + \frac{T^2}{12}(2N^3 - 3N^2 + N) + \frac{T^3}{24}(N^4 - 2N^3 + N^2) + \ldots \] (29)
Keeping terms up to first order in $T$, the Hamiltonian of Eq. (27) can be written as

$$H = N_1 \left(1 - \frac{T}{2}\right) + \frac{T}{2} N_1^2 + N_2 \left(1 - \frac{T}{2}\right) + \frac{T}{2} N_2^2 + T N_1 N_2 + \ldots \quad (30)$$

The first two terms in this expansion describe an anharmonic oscillator of the Morse type with self-anharmonicity $^{35}$

$$x = \frac{T/2}{1 - T/2}. \quad (31)$$

The third and fourth terms in Eq. (30) describe another Morse oscillator with the same self-anharmonicity. The last term in Eq. (30) describes the cross-anharmonicity between the two Morse oscillators, imposed by the overall su$_Q$(2) symmetry. The cross-anharmonicity is of the same type as the one encountered in the empirical Eqs (1) and (2).

We conclude therefore that the system of two $Q$-oscillators coupled so that the total system has the su$_Q$(2) symmetry is equivalent to the system of two coupled Morse oscillators usually used for the description of vibrational spectra of triatomic molecules.

The fact that $Q$-oscillators turn out to be suitable for the description of molecules, while $q$-oscillators do not, can be traced back to the physical content of these oscillators. It has been found that the $Q$-oscillators correspond to WKB equivalent potentials which are harmonic oscillator potentials with $x^4$ perturbations$^{36}$, while the $q$-oscillators correspond to WKB equivalent potentials which are harmonic oscillator potentials with $x^6$ perturbations$^{12}$. The relation between the $Q$-oscillators and the Morse potential (which is also a harmonic oscillator potential with leading $x^4$ perturbations) has also been clarified $^{37}$.

This construction can be easily generalized to the case of $l$ coupled $Q$-oscillators, having the su$_Q(l)$ overall symmetry. The Hamiltonian then reads

$$H = [N_1 + N_2 + \ldots + N_l]_Q. \quad (32)$$

In order to discuss the physical content of this Hamiltonian, we write explicitly the result for the case with $l = 3$, using the Taylor expansion of Eq. (29) and keeping terms only up to first order in $T$

$$H(N_1, N_2, N_3) = \sum_{i=1}^{3} \left(1 - \frac{T}{2}\right) N_i + \frac{T}{2} N_i^2 + T(N_1 N_2 + N_2 N_3 + N_3 N_1). \quad (33)$$
We remark that the result is three identical oscillators with self-anharmonicity given by Eq. (31) and coupled by cross-anharmonic terms of the type $N_iN_j$ multiplied by the same strength $T$. It is worth recalling that this situation is realized in highly symmetric molecules, such as benzene \textsuperscript{21–23} and the octahedral XY\textsubscript{6} molecules treated in \textsuperscript{20}. In these molecules all bonds are equivalent and all diagonal cross-anharmonicities among them have the same strength, as implied by the $\text{su}_Q(l)$ ($\text{su}_Q(3)$) symmetry in Eq. (32) (Eq. (33)).

In Eq. (30) it is clear that the cross-anharmonicity strength $T$ and the self-anharmonicity of the oscillators $x$ are connected as described by Eq. (31). This connection is imposed by the symmetry used. Such constraints (imposed by symmetries) between the parameters can be useful in reducing the total number of free parameters in a model, as pointed out in \textsuperscript{38}. Similar constraints appear in the case of the vibron model, where they have been found particularly useful in reducing the total number of free parameters when dealing with four-atomic or larger molecules \textsuperscript{39}. In order to have larger flexibility, though, one might wish to avoid the connection imposed by Eq. (31). This can be achieved through the use of generalized deformed oscillators \textsuperscript{11} (deformed anharmonic oscillators) of the form

$$H_i = [N_i + c_iN_i^2]Q. \quad (34)$$

(Such oscillators have already been successfully used for the description of vibrational spectra of diatomic molecules \textsuperscript{11}.) Two of these oscillators can be coupled in a way similar to that described by Eq. (28), giving

$$H(N_1, N_2) = [N_1 + c_1N_1^2]Q\frac{Q^{N_2+c_2N_2^2} + 1}{2} + \frac{Q^{N_1+c_1N_1^2} + 1}{2}[N_2 + c_2N_2^2]Q$$

$$= [N_1 + c_1N_1^2 N_2 + c_2N_2^2]Q. \quad (35)$$

Using the Taylor expansion of Eq. (29) and keeping terms only up to first order in $T$, we have

$$H(N_1, N_2) = (N_1 + c_1N_1^2) \left(1 - \frac{T}{2}\right) + \frac{T}{2}(N_1^2 + 2c_1N_1^3 + c_1^2N_1^4)$$

$$\quad + (N_2 + c_2N_2^2) \left(1 - \frac{T}{2}\right) + \frac{T}{2}(N_2^2 + 2c_2N_2^3 + c_2^2N_2^4)$$

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\( + T(N_1 N_2 + c_1 N_1^2 N_2 + c_2 N_1 N_2^2 + c_1 c_2 N_1^2 N_2^2). \)  

(36)

The physical content of this equation is clear. The first two terms describe an oscillator with self-anharmonicity (defined as the ratio of the coefficient of the \( N_i^2 \) term over that of the \( N_i \) term)

\[ x_1 = c_1 + \frac{T/2}{1 - T/2}, \]  

(37)

the third and fourth terms describe an oscillator with self-anharmonicity

\[ x_2 = c_2 + \frac{T/2}{1 - T/2}, \]  

(38)

while the leading cross-anharmonicity between the two oscillators, contained in the fifth term, is \( T N_1 N_2 \). Therefore Eq. (36) describes to lowest order two Morse oscillators coupled by the lowest order cross-anharmonicity usually used empirically.

Several comments are now in place:

i) From comparisons to experimental data of diatomic molecules it is known \(^{11} \) that \( T \) and \( c_i \) are small. Therefore their present use as small parameters is justified. In particular it is known that in general \( c_i N_i \ll 1 \), so that the terms cubic and quartic in \( N_i \) occurring in Eq. (36) are of magnitude smaller than the corresponding leading terms which are quadratic in \( N_i \).

ii) In Eq. (36) the connection between the self-anharmonicity constants and the cross-anharmonicity strength is destroyed, as wished. The \( Q \)-deformation is connected to the cross-anharmonicity strength \( T \), while its effect on the self-anharmonicity constants, seen in Eqs. (37) and (38), is a simple renormalization.

iii) In Eq. (36) the two oscillators are characterized by different self-anharmonicities, given by Eqs (37) and (38). This is a feature needed in several molecules in which one has to treat inequivalent vibrational modes. It is clear that oscillators with different self-anharmonicities occur only in the case of the generalized deformed oscillators used in Eq. (36) and not in the case of the \( Q \)-oscillators used in Eq. (30).

iv) The generalization of Eq. (35) to \( l \) oscillators reads

\[ H(N_1, N_2, \ldots, N_l) = [N_1 + c_1 N_1^2 + N_2 + c_2 N_2^2 + \ldots + N_l + c_l N_l^2]_Q. \]  

(39)
Using the Taylor expansion of Eq. (29) it is clear that to lowest order \( l \) Morse oscillators with self-anharmonicities similar to the ones of Eqs (37), (38) are obtained, while the cross-anharmonicities among them are of the \( TN_iN_j \) type.

v) In highly symmetric molecules, such as benzene \(^{21-23}\) and the octahedral \( XY_6 \) molecules used in \(^{20}\), all bonds are equivalent. Therefore in Eq. (39) one should use \( c_1 = c_2 = \ldots c_l \). In these molecules the diagonal cross-anharmonicities among the various bonds are also of the same type \(^{20-23}\), therefore the occurrence of the common coefficient \( T \) in front of the cross-anharmonic terms \( N_iN_j \) is justified.

vi) Eq. (35) clearly shows that comultiplication is absent in this extended model, even in the case with \( c_1 = c_2 \). (For comultiplication to be present, one should have obtained \( c(N_1 + N_2)^2 \) instead of \( cN_1^2 + cN_2^2 \) in the last term of Eq. (35).) Thus the Hopf algebraic structure, which is present in the Hamiltonians of Eqs (27) and (32), is lost in the case of the Hamiltonian of Eq. (35).

vii) In order to obtain better agreement with the data, one has to add to the Hamiltonians of Eqs. (1), (2) non-diagonal interaction terms of the form \(^{17,18}\)

\[
H_{ij} = a_i^\dagger a_j + a_j^\dagger a_i.
\]  

Such terms are also used by the Iachello and Oss approach \(^{20-23,40}\). Alternatively, terms introducing Darling–Dennison couplings \(^{16}\)

\[
H_{ij}^{DD} = a_i^\dagger a_i^\dagger a_j a_j + a_j^\dagger a_j^\dagger a_i a_i
\]  

can be used \(^{19,40}\). It is clear that such terms are not contained in the Hamiltonians of Eqs (27), (32), (35), (39) considered here. The matrix elements of such operators can be calculated in a straightforward way. For example, the matrix elements of a term \( b_i^\dagger b_j \) added to the Hamiltonian of Eq. (27) are

\[
< n_i + 1, n_j - 1|b_i^\dagger b_j|n_i, n_j > = \sqrt{[n_i + 1]_Q[n_j]_Q},
\]  

because of Eq. (20). Similarly one has

\[
< n_i + 2, n_j - 2|b_i^\dagger b_i^\dagger b_j b_j|n_i, n_j > = \sqrt{[n_i + 2]_Q[n_i + 1]_Q[n_j]_Q[n_j - 1]_Q}.
\]
viii) An algebraic model based on two coupled anharmonic vibrations for the description of ABA triatomics has been developed in \( ^{41} \). The diagonal part of its Hamiltonian can be rewritten in the form of Eq. (2), involving three free parameters. To leading order it is then equivalent to Eq. (36) of the present formalism, which contains the same leading terms and involves three free parameters as well.

In summary, we have proved that a system of \( n \) \( Q \)-deformed oscillators coupled so that the total Hamiltonian is characterized by the \( \text{su}_Q(n) \) symmetry is equivalent, to lowest order approximation, to a system of \( n \) identical Morse oscillators coupled by the cross-anharmonicity usually used empirically in the description of vibrational spectra of polyatomic molecules. This symmetry also implies a relation between the self-anharmonicity of the Morse oscillators and the cross-anharmonicity strength, which can be avoided by replacing the \( Q \)-oscillators by deformed anharmonic oscillators (generalized deformed oscillators), at the cost of losing the Hopf algebraic structure. No Darling–Dennison or other nondiagonal interaction terms are contained in this scheme. For introducing such terms in the quantum algebraic framework the approach of \(^{40}\) can be used.

**Acknowledgement**

One of the authors (DB) has been supported by the EU under contract ERBCHBGCT930467.
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