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Model of n coupled generalized deformed oscillators for vibrations of polyatomic molecules

Dennis Bonatsos*
Institute of Nuclear Physics, National Center for Scientific Research, "Demokritos,"
GR-15310 Aghia Paraskevi, Attiki, Greece

C. Daskaloyannis†
Theoretical Physics Department, Aristotle University of Thessaloniki, GR-54006 Thessaloniki, Greece

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A generalized deformed oscillator giving the same spectrum as the Morse potential is constructed through the use of quantum-algebraic techniques. The model of n coupled anharmonic oscillators of Iachello and Oss [Phys. Rev. Lett. **66**, 2976 (1991)], suitable for the description of vibrational spectra of polyatomic molecules, is subsequently written in terms of such generalized deformed oscillators. In addition to clarifying the relation of the model of Iachello and Oss to other models using coupled oscillators for the description of vibrational molecular spectra, the present formalism allows for the construction of a large class of exactly soluble models with no extra computational effort. As an example, the way of including a coupling of the Darling-Dennison type is shown.

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I. INTRODUCTION

Quantum algebras (also called quantum groups) [1–4] are receiving recently much attention in physics. From the mathematical point of view they are q deformations of the universal enveloping algebras of the corresponding Lie algebras. When the deformation parameter q is set equal to 1, the usual Lie algebras are obtained. Quantum algebras are concrete examples of Hopf algebras [3, 4]. Initially used for solving the quantum Yang-Baxter equation [5], they are now finding applications in several branches of physics, especially after the introduction of the q-deformed harmonic oscillator [6, 7]. Applications in conformal field theory [8], quantum gravity [9], quantum optics [10], nuclear physics [11, 12], as well as in the description of spin chains [13] have already appeared, while in atomic physics attention has been focused on the hydrogen atom [14, 15].

Rotational spectra of diatomic molecules [16, 17], deformed nuclei [18, 19], and superdeformed nuclei [20] have been described in terms of the q-deformed rotator having the symmetry $\mathrm{SU}_q(2)$, the deformation parameter τ^2 (with $q = e^{i\tau}$) found [19] to correspond to the softness parameter of the variable moment of inertia model. The implications of the $\mathrm{SU}_q(2)$ symmetry on the electric transition probabilities connecting the rotational levels have also been studied [21]. Vibrational spectra of diatomic molecules have been described in terms of q-deformed harmonic [22–25] and anharmonic [26, 27] oscillators having the $\mathrm{SU}_q(1,1)$ symmetry. WKB equivalent potentials for these oscillators have been determined [28, 29], the WKB equivalent potential corresponding to the $\mathrm{SU}_q(1,1)$ symmetry found [29] to be a deformation of the modified Pöschl-Teller potential, which is connected to the Morse potential by a known transformation [30].

On the other hand, a powerful method for the algebraic description of vibrational spectra of polyatomic molecules has been recently introduced by Iachello and Oss [31–33]. In this method, each bond in a polyatomic molecule is replaced by a Morse oscillator. The model is obviously superior in comparison to models attempting the description of vibrational spectra of polyatomic molecules in terms of coupled harmonic oscillators [34–37], since it incorporates anharmonicities in a natural way. It is also much easier to use than the vibron model [38, 39], in which rotations and vibrations are treated simultaneously.

Since it is by now understood that the q-deformed oscillator is also a case of an anharmonic oscillator [40], it is reasonable to try to construct creation and annihilation operators describing a Morse oscillator, in a way similar to the description of the usual harmonic oscillator in the occupation number representation ("second quantization"). These operators can then be used in formulating the model of n coupled anharmonic oscillators of Iachello and Oss [31–33] in terms of deformed oscillators.

In this paper first we are going to construct creation and annihilation operators giving the same spectrum as the Morse potential. Subsequently, the model of n coupled anharmonic oscillators of Iachello and Oss will be written in terms of these oscillators. In this way the relation of this model to existing models using coupled oscillators for the description of vibrational spectra of polyatomic molecules [34–37] will be clarified. Furthermore, it will be demonstrated how a large class of exactly soluble models for the description of vibrations of polyatomic molecules can be constructed with no extra computational effort, by taking advantage of the freedom in the choice of the deformed oscillators involved and the simplicity of the occupation number representation formalism.

In Sec. II of this paper a generalized deformed oscillator giving the same spectrum as the Morse potential will be constructed, while in Sec. III the model of n coupled anharmonic oscillators of Iachello and Oss will be written in terms of such generalized deformed oscillators, its relation to existing models will be examined, and the construction of additional exactly soluble models will be discussed. Finally, in Sec. IV discussion of the present results and plans for further work will be given.

II. A GENERALIZED DEFORMED OSCILLATOR FOR THE MORSE POTENTIAL

Solving the Schrödinger equation for the Morse potential [31, 41, 42]

$$V(x) = D\left(1 - e^{-\alpha x}\right)^2, \tag{1}$$

one obtains the energy spectrum

$$E(v) = -D - 4A(\mathcal{N} v - v^2), \tag{2}$$

where

$$v = 0, 1, \ldots, \frac{\mathcal{N}}{2} \quad \text{or} \quad \frac{\mathcal{N}-1}{2} \tag{3}$$

(where $\mathcal{N}$ is even or odd) and

$$-4A\mathcal{N} = \hbar\alpha\sqrt{\frac{2D}{m}}, \qquad 4A = -\frac{\hbar^2\alpha^2}{2m}. \tag{4}$$

The anharmonicity constant $x_e = 1/\mathcal{N}$, defined by Cooper [43], is a perturbational parameter for the Morse potential, measuring the deviation from the harmonic-oscillator limit, which is obtained at $x_e \to 0$.

Our first aim is to construct a deformed oscillator giving the same spectrum as in Eq. (2). Deformed oscillators giving the spectrum of a Pöschl-Teller potential have already been studied in [44], where the method of [45] was applied. This method gives the deformed oscillator directly from the energy spectrum. The Pöschl-Teller spectrum coincides with the spectrum of the Morse potential up to an energy shift, therefore the oscillator algebra of [44] can be transferred to the case of the Morse potential.

A general deformation of the harmonic oscillator can be given by the basic relation [45]

$$f(aa^\dagger) - f(a^\dagger a) = 1, \tag{5}$$

where $a^\dagger$ (a) are creation (annihilation) operators and $f(x)$ is a real analytic function defined on the real positive axis. In the case of the usual harmonic oscillator one has $f(x) = x$, which leads to the usual boson commutation relation $[a, a^\dagger] = 1$.

The number operator N satisfies, by definition, the commutation relations

$$[a, N] = a, \quad [a^\dagger, N] = -a^\dagger. \tag{6}$$

It can be shown [45] that

$$N = f(a^\dagger a). \tag{7}$$

If (5) holds, then it is also true that

$$aa^\dagger = g(a^\dagger a), \tag{8}$$

where the function $g(x)$ is defined by

$$g(x) = F(1 + f(x)), \quad F = f^{-1}. \tag{9}$$

If $|\alpha\rangle$ is a base of eigenvectors of the number operator N

$$N|\alpha\rangle = \alpha|\alpha\rangle, \tag{10}$$

then from Eq. (6) one has

$$a|\alpha\rangle = \sqrt{[\alpha]}|\alpha - 1\rangle, \quad a^\dagger|\alpha\rangle = \sqrt{[\alpha+1]}|\alpha + 1\rangle, \tag{11}$$

where $[\alpha]$ is a function of α. Furthermore from Eq. (9) one has

$$[\alpha + 1] = g([\alpha]) \quad \text{or} \quad f([\alpha + 1]) = 1 + f([\alpha]), \tag{12}$$

from which we conclude that [45]

$$[\alpha] = F(\alpha). \tag{13}$$

The eigenvector $|0\rangle$, corresponding to the zero eigenvalue of the number operator N, satisfies the following relation

$$\text{if} \quad F(0) = 0 \quad [\text{or} \quad f(0) = 0], \quad \text{then} \quad a|0\rangle = 0. \tag{14}$$

In this paper we assume that the function $F(x)$ is zero when $x = 0$.

The number operator N defined by Eq. (7) satisfies Eqs. (6). The following identities are also useful:

$$a^\dagger a = F(N) = [N], \qquad aa^\dagger = F(N+1) = [N+1], \tag{15}$$

and

$$[a, a^\dagger] = [N+1] - [N], \qquad \{a, a^\dagger\} = [N+1] + [N]. \tag{16}$$

If $h(z)$ is an entire function, then the following properties are true:

$$h(N)\left(a^\dagger\right)^m = \left(a^\dagger\right)^m h(N+m), \tag{17}$$

$$h(N+m)\left(a\right)^m = \left(a\right)^m h(N). \tag{18}$$

The eigenvectors of the number operator N are generated by the formula

$$|n\rangle = \frac{1}{\sqrt{[n]!}}(a^\dagger)^n|0\rangle, \tag{19}$$

where

$$[n]! = \prod_{k=1}^{n}[k] = \prod_{k=1}^{n} F(k). \tag{20}$$

These eigenvectors are also eigenvectors of the energy operator

$$H = \frac{A}{2}(aa^\dagger + a^\dagger a), \tag{21}$$

corresponding to the eigenvalues

$$E_n = \frac{A}{2}([n+1]+[n]) = \frac{A}{2}[F(n+1)+F(n)]. \tag{22}$$

If the energy spectrum is given by a definite real function of the number $n+1/2$

$$E_n = \frac{A}{2}H(n+\tfrac{1}{2}), \tag{23}$$

then

$$H(x+\tfrac{1}{2}) = \tfrac{1}{2}[F(x+1)+F(x)]. \tag{24}$$

The specific properties of the generalized deformed oscillator formulated above are fixed by the structure function $F(n)$. By choosing

$$F(n) = n, \tag{25}$$

one obtains the usual harmonic oscillator. For

$$F(n) = \frac{q^n - q^{-n}}{q - q^{-1}} = [n], \tag{26}$$

one obtains the q-deformed harmonic oscillator of Biedenharn [6] and Macfarlane [7], while by selecting

$$F(n) = \frac{Q^n - 1}{Q - 1} \tag{27}$$

the Q-deformed oscillator of Arik and Coon [46] can be generated. For $Q > 1$ the spectrum of this oscillator increases more rapidly than the equidistant spectrum of the usual harmonic oscillator, while for $Q < 1$ its spectrum increases less rapidly than the equidistant one, i.e. it is compressed, bearing similarity to the spectrum of the Morse oscillator.

We now look for a structure function which will give a spectrum similar to that of Eq. (2). Since Eq. (2) contains a polynomial quadratic in v and in addition we wish to keep $F(0) = 0$, the structure function should be of the form

$$F(V) = a_1 V + b_1 V^2. \tag{28}$$

Using Eqs. (2) and (24) we easily conclude that a solution to the problem is provided by the structure function

$$F(V) = V(\mathcal{N}+1-V). \tag{29}$$

Using the basis $|\mathcal{N}, v\rangle$ of eigenfunctions of the "number operator" V, one has in the place of Eqs. (10) and (11) the relations

$$V|\mathcal{N}, v\rangle = v|\mathcal{N}, v\rangle, \tag{30}$$

$$\begin{aligned} a|\mathcal{N}, v\rangle &= \sqrt{F(v)}|\mathcal{N}, v-1\rangle, \\ a^{\dagger}|\mathcal{N}, v\rangle &= \sqrt{F(v+1)}|\mathcal{N}, v+1\rangle. \end{aligned} \tag{31}$$

The structure function of Eq. (28) leads then to a spectrum

$$\begin{aligned} E'(v) &= -4A\left(\frac{F(v)+F(v+1)}{2}\right) \\ &= -4A(\mathcal{N}v - v^2) - 2A\mathcal{N}. \end{aligned} \tag{32}$$

Then Eq. (2) can be written in the form

$$E(v) = E'(v) + 2A\mathcal{N} - D, \tag{33}$$

i.e., the spectrum of the generalized deformed oscillator constructed here is the same as the spectrum of the Morse potential up to an additive constant.

III. MODEL OF n COUPLED GENERALIZED DEFORMED OSCILLATORS

Iachello and Oss [31–33] introduced recently a model of n coupled anharmonic oscillators for the description of vibrational spectra of polyatomic molecules. In this model each bond i in a polyatomic molecule is replaced by a Morse oscillator. The model Hamiltonian has the form

$$H = E_0 + \sum_{i=1}^{n} A_i C_i + \sum_{\substack{i=1 \\ i<j}}^{n} A_{ij} C_{ij} + \sum_{\substack{i=1 \\ i<j}}^{n} \lambda_{ij} M_{ij}, \tag{34}$$

where C_i gives the spectrum of the ith Morse oscillator, while the interactions among the various Morse oscillators are described by C_{ij} and M_{ij}, the Casimir and Majorana interactions, respectively. The eigenvalues of C_i in the basis $|\mathcal{N}_i, v_i\rangle$ are given by

$$\langle \mathcal{N}_i, v_i | C_i | \mathcal{N}_i, v_i \rangle = -4(\mathcal{N}_i v_i - v_i^2). \tag{35}$$

The Casimir interaction C_{ij} is diagonal in the basis $|\mathcal{N}_i, v_i, \mathcal{N}_j, v_j\rangle$, its matrix elements being

$$\begin{aligned} &\langle \mathcal{N}_i, v_i, \mathcal{N}_j, v_j | C_{ij} | \mathcal{N}_i, v_i, \mathcal{N}_j, v_j \rangle \\ &\qquad = 4[(v_i+v_j)^2 - (v_i+v_j)(\mathcal{N}_i+\mathcal{N}_j)], \end{aligned} \tag{36}$$

while the Majorana interaction M_{ij} has diagonal matrix elements

$$\langle \mathcal{N}_i, v_i, \mathcal{N}_j, v_j | M_{ij} | \mathcal{N}_i, v_i, \mathcal{N}_j, v_j \rangle = v_i \mathcal{N}_j + v_j \mathcal{N}_i - 2 v_i v_j \tag{37}$$

and nondiagonal matrix elements

$$\begin{aligned} &\langle \mathcal{N}_i, v_i+1, \mathcal{N}_j, v_j-1 | M_{ij} | \mathcal{N}_i, v_i, \mathcal{N}_j, v_j \rangle \\ &\qquad = -\sqrt{u_j(v_i+1)(\mathcal{N}_i - v_i)(\mathcal{N}_j - v_j + 1)}, \end{aligned} \tag{38}$$

$$\begin{aligned} &\langle \mathcal{N}_i, v_i-1, \mathcal{N}_j, v_j+1 | M_{ij} | \mathcal{N}_i, v_i, \mathcal{N}_j, v_j \rangle \\ &\qquad = -\sqrt{v_i(v_j+1)(\mathcal{N}_j - v_j)(\mathcal{N}_i - v_i + 1)}. \end{aligned} \tag{39}$$

We are now going to express these results in terms of the generalized deformed oscillator equivalent to the Morse potential, introduced in the previous section. Having in mind that

$$a_i^{\dagger} a_i = F(V_i), \qquad a_i a_i^{\dagger} = F(V_i+1), \tag{40}$$

and noticing that

$$\{a_i, a_i^\dagger\}|\mathcal{N}_i, v_i\rangle = [F(V_i+1) + F(V_i)]|\mathcal{N}_i, v_i\rangle$$
$$= (2\mathcal{N}_i v_i - v_i^2 + \mathcal{N}_i)|\mathcal{N}_i, v_i\rangle, \qquad (41)$$

it is clear that the operator

$$C_i = 2(\mathcal{N}_i - \{a_i, a_i^\dagger\}) = 2[\mathcal{N}_i - F(V_i) - F(V_i+1)], \qquad (42)$$

has the eigenvalues given in Eq. (35).

Our next aim is to express the Casimir operator C_{ij} in terms of generalized oscillators. Noticing that

$$[a_i, a_i^\dagger]|\mathcal{N}_i, v_i\rangle = [F(V_i+1) - F(V_i)]|\mathcal{N}_i, v_i\rangle$$
$$= (\mathcal{N}_i - 2v_i)|\mathcal{N}_i, v_i\rangle, \qquad (43)$$

$$[a_i, a_i^\dagger][a_j, a_j^\dagger]|\mathcal{N}_i, v_i, \mathcal{N}_j, v_j\rangle = [F(V_i+1) - F(V_i)][F(V_j+1) - F(V_j)]|\mathcal{N}_i, v_i, \mathcal{N}_j v_j\rangle$$
$$= (\mathcal{N}_i - 2v_i)(\mathcal{N}_j - 2v_j)|\mathcal{N}_i, v_i, \mathcal{N}_j, v_j\rangle, \qquad (44)$$

it is easy to verify that the operator

$$C_{ij} = 2(\mathcal{N}_i - \{a_i, a_i^\dagger\} + \mathcal{N}_j - \{a_j, a_j^\dagger\} - \mathcal{N}_i\mathcal{N}_j + [a_i, a_i^\dagger][a_j, a_j^\dagger]), \qquad (45)$$

has the matrix elements given in Eq. (36).

Finally, we wish to express the Majorana operator M_{ij} in terms of generalized oscillators. Noticing that

$$a_i^\dagger a_j|\mathcal{N}_i, v_i, \mathcal{N}_j, v_j\rangle = \sqrt{F(V_i+1)F(V_j)}|\mathcal{N}_i, v_i+1, \mathcal{N}_j, v_j-1\rangle$$
$$= \sqrt{(v_i+1)(\mathcal{N}_i - v_i)v_j(\mathcal{N}_j - v_j + 1)}|\mathcal{N}_i, v_i+1, \mathcal{N}_j, v_j-1\rangle, \qquad (46)$$

and using Eq. (44) it is easy to verify that the operator

$$M_{ij} = -a_i^\dagger a_j - a_j^\dagger a_i - \frac{1}{2}[a_i, a_i^\dagger][a_j, a_j^\dagger] + \frac{1}{2}\mathcal{N}_i\mathcal{N}_j, \qquad (47)$$

has the matrix elements given in Eqs. (37)–(39).

Using Eqs. (42), (45) and (47), the Hamiltonian of Eq. (34) can then be written as

$$H = E_0' + \sum_{i=1}^{n} A_i'\{a_i, a_i^\dagger\} + \sum_{i<j}^{n} A_{ij}'[a_i, a_i^\dagger][a_j, a_j^\dagger]$$
$$+ \sum_{i<j}^{n} \lambda_{ij}'(a_i^\dagger a_j + a_j^\dagger a_i), \qquad (48)$$

where the constants E_0',A_i',A_{ij}', λ_{ij}' can be easily expressed in terms of the constants E_0,A_i,A_{ij},λ_{ij} of Eq. (34) and $\mathcal{N}_i$, $\mathcal{N}_j$.

A few comments are now in order.

(i) The Hamiltonian of Eq. (48) is fully equivalent to the one of Iachello and Oss [Eq. (34)], when the generalized deformed bosons used in it are characterized by the structure function of Eq. (29). However, the present formalism can be also used with generalized deformed bosons characterized by other structure functions related to vibrational molecular spectra. Thus the present formalism offers as a bonus a large number of exactly soluble models at no further computational cost.

(ii) An exactly soluble model [as an example of comment (i)] can be obtained by using the structure function

$$F(N) = [N + b\gamma], \qquad (49)$$

where the brackets indicate the usual q numbers of Eq. (26). This structure function has been used by Chang and Yan for the description of vibrational molecular spectra in [22, 23]. If γ is allowed to be an appropriate function of the angular momentum J, a description of both rotational and vibrational molecular spectra is obtained [24, 25]. For $b = 0$ the usual q-deformed harmonic oscillator [6, 7] is obtained.

(iii) Another example of exactly soluble model, according to (i), is given by the structure function [47]

$$F(N) = [N + cN^2], \qquad (50)$$

where again the brackets indicate the usual q numbers of Eq. (26). For $q = 1$ the brackets go away and this structure function is equivalent to the one characterizing the Morse potential [Eq. (29)], used here. For $q \neq 1$ this structure function represents a q deformation of the Morse potential, an approach alternative to the use of a potential described by an expansion in terms of Morse functions. It should be recalled at this point that improved descriptions of vibrational spectra of diatomic molecules have been obtained in terms of q-deformed anharmonic oscillators having the $\mathrm{U}_q(2) \supset \mathrm{O}_q(2)$ [26] and $\mathrm{SU}_q(1,1)$ [27] symmetries. WKB equivalent potentials giving the same spectrum as these q-deformed anharmonic oscillators have been obtained in [29]. They are q-deformed versions of the modified Pöschl-Teller potential, which is connected to the Morse potential by a known transformation [30]. It is therefore clear that the need for q-deformed versions of the Morse potential occurs in these cases as well.

(iv) In the case of polyatomic molecules having specific symmetries, such as the benzene [32, 33] or octahedral XY_6 molecules [31], the coefficients in Eq. (48) get simplified, since the arguments used in Refs. [31–33] are still valid. In the two examples just mentioned (benzene, octahedral molecules), all bonds are equivalent, so that $\mathcal{N}_i = \mathcal{N}$, $A'_i = A'$ for any i, $A'_{ij} = B$ for any i and j. For the off-diagonal couplings, described by the last term in Eq. (48), different cases have to be considered. In the case of octahedral XY_6 molecules, for example, one has to distinguish between adjacent and opposite bonds, as in [31], while in the case of benzene nearest-neighbor couplings, next to nearest-neighbor couplings and opposite bond couplings, as in [32, 33], have to be considered.

(v) The expression of the model of n coupled anharmonic oscillators of Iachello and Oss in terms of generalized deformed oscillators is also helpful in clarifying the connection between the present model and earlier models using coupled oscillators for the description of molecular vibrations. The usual Hamiltonian for the description of vibrational modes of polyatomic molecules reads [34]

$$H = \sum_i \omega_i \left(v_i + \frac{d_i}{2} \right) + \sum_i \sum_{k \geq i} x_{ik} \left(v_i + \frac{d_i}{2} \right) \left(u_k + \frac{d_k}{2} \right), \tag{51}$$

where d_i,d_k are the degeneracies of the corresponding modes. It is clear that the first term of the Hamiltonian of Eq. (51), as well as the parts of the second term with $i = k$, are equivalent to the second term in Eq. (48), while the parts of the second term of Eq. (51) with $k > i$ are included in the third term of Eq. (48).

(vi) Another example is provided by the Hamiltonian of Kellman [35]

$$H = (a_1^\dagger a_1 + a_2^\dagger a_2 + 1) \left(1 + \frac{1}{M} \right) - \frac{1}{M} (a_1^\dagger a_2 + a_2^\dagger a_1), \tag{52}$$

which is included in the first, second, and fourth terms of Eq. (48).

(vii) Another Hamiltonian by Kellman [36]

$$H = \hbar\omega_0 (n_1 + n_2 + 1) + \frac{\alpha}{2} [(n_1 + \tfrac{1}{2})^2 + (n_2 + \tfrac{1}{2})^2] + \alpha_{12} (n_1 + \tfrac{1}{2})(n_2 + \tfrac{1}{2}) + \frac{\beta}{2} (a_1^\dagger a_2 + a_2^\dagger a_1), \tag{53}$$

used for the description of vibrational spectra of ABA triatomic molecules, is also a special case of Eq. (48). In particular, the first two terms of the Hamiltonian of Eq. (53) are contained in the second term of the Hamiltonian of Eq. (48), while the third (fourth) term of Eq. (53) corresponds to the third (fourth) term of Eq. (48).

(viii) Kellman has also used for the description of ABA triatomic molecules the Hamiltonian [37]

$$H = \hbar\omega_s (n_s + \tfrac{1}{2}) + \hbar\omega_a (n_a + \tfrac{1}{2}) + \frac{\gamma_s}{2} (n_s + \tfrac{1}{2})^2 + \frac{\gamma_a}{2} (n_a + \tfrac{1}{2})^2 + \gamma_{sa} (n_s + \tfrac{1}{2})(n_a + \tfrac{1}{2}) + \delta (a_s^\dagger a_s^\dagger a_a a_a + a_a^\dagger a_a^\dagger a_s a_s), \tag{54}$$

of which the first four terms are equivalent to the second term of Eq. (48), while its fifth term is contained in the third term of Eq. (48). The last term of the Hamiltonian of Eq. (54) is not contained in Eq. (48). This term is suitable for reproducing the Darling-Dennison normal-mode coupling [48]. In the case of the exactly soluble models expressed by the Hamiltonian of Eq. (48), it is a trivial task to include such a term. The corresponding matrix elements are then

$$\langle \mathcal{N}_i, v_i + 2, \mathcal{N}_j, v_j - 2 | a_i^\dagger a_i^\dagger a_j a_j | \mathcal{N}_i, v_i, \mathcal{N}_j, v_j \rangle = \sqrt{F(v_i + 2) F(v_i + 1) F(v_j) F(v_j - 1)}. \tag{55}$$

For simple (not deformed) oscillators, for which $F(v_i) = v_i$, eq. (55) gives the Darling-Dennison result, while in the case of generalized deformed (anharmonic) oscillators the Darling-Dennison coupling is the lowest-order term in an expansion using the anharmonicity constants as small parameters.

(ix) A Hamiltonian recently treated is [49]

$$H = a_0 I + b_0 \sum_{i=1}^{d} a_i^\dagger a_i + c_0 \sum_{i,j=1 (i<j)}^{d} (a_i^\dagger a_j + a_j^\dagger a_i) + d_0 \sum_{i=1}^{d} [(a_i^\dagger)^2 + a_i^2] + c_0 \sum_{i,j=1 (i<j)}^{d} (a_i^\dagger a_j^\dagger + a_i a_j), \tag{56}$$

the second (third) term of which is contained in the second (fourth) term of the Hamiltonian of Eq. (48), while its fourth and fifth terms are not included in Eq. (48).

IV. DISCUSSION

In this paper a generalized deformed oscillator giving the same spectrum as the Morse potential was first constructed. Subsequently, the model of n coupled anharmonic oscillators of Iachello and Oss [31–33] was written in terms of such generalized oscillators. In addition to clarifying the relation of the model to existing models using coupled oscillators for the description of vibrational spectra of diatomic molecules [34–37, 49], the present formalism allows for the construction of a large class of exactly soluble models with no extra computational effort. As an example, the way of including a term giving the Darling-Dennison coupling has been demonstrated.

Applications of some of the above-mentioned exactly soluble models to vibrational spectra of specific polyatomic molecules should be carried out in order to check the relative significance of the various contributing terms.

The spectrum of the q-deformed harmonic oscillator can be also obtained from solving the q-deformed Schrödinger equation [50] for the usual harmonic oscillator potential. The q-deformed Schrödinger equation for the hydrogen atom has also been studied recently [15]. It will be interesting to construct the q-deformed Schrödinger equation for the Morse potential and check the changes inflicted by the q-deformation on the spectrum. It will also be of interest to construct the q-deformed Schrödinger equation for the modified Pöschl-Teller potential and check the relation between its eigenvalues and the spectrum of the q-deformed anharmonic oscillator with $SU_q(1,1)$ symmetry of Ref. [27], for which the WKB equivalent potential has been shown [29] to be a q deformation of the usual modified Pöschl-Teller potential. The q-deformed version of the vibron model [38, 39] of molecular structure as well as of the interacting boson model of nuclear structure ([51]; see [52, 53] for recent overviews) are also of interest; a step in this direction has been taken already in [54]. Work in these directions is in progress.

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* Electronic address: bonat@isosun.ariadne-t.gr
† Electronic address: cabz03@grtheun1.bitnet

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