Eur. Phys. J. D **40**, 205–210 (2006)
DOI: 10.1140/epjd/e2006-00155-6

**THE EUROPEAN
PHYSICAL JOURNAL D**

A method based on a nonlinear generalized Heisenberg algebra to study the molecular vibrational spectrum

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Received 30 December 2005 / Received in final form 12 May 2006

Abstract. We propose a method, based on a generalized Heisenberg algebra (GHA), to reproduce the anharmonic spectrum of diatomic molecules. The theoretical spectrum generated by GHA allows us to fit the experimental data and to obtain the dissociation energy for the carbon monoxide molecule. Our outcomes are more accurate than the standard models used to study molecular vibrations, namely the Morse and the q-oscillator models and comparable to the perturbed Morse model proposed by Huffaker [1], for the first experimental levels. The dissociation energy obtained here is more accurate than all previous models.

PACS. 33.20.Tp Vibrational analysis – 02.20.Uw Quantum groups – 03.65.Fd Algebraic methods – 32.30.Bv Radio-frequency, microwave, and infrared spectra

1 Introduction

Vibrational spectroscopy has a fundamental role in molecular physics and its applications extend to other fields like astronomy [2], biology [3] and earth and environmental sciences [4]. Vibrational molecular analysis provides important informations on the structure of the molecules. Recently, the development of the powerful experimental techniques allow the study of highly excited vibrational states [5,6]. In Born-Oppenheimer approximation, electronic, rotational and vibrational quantum states [3] can be considered separately and molecular vibrations can be approximately described by the harmonic oscillator [7]. However, this model fails to describe the highest molecular vibrational modes and consequently does not provide the correct dissociation energies. One of the first models that introduce a correction in the harmonic term, was proposed by Morse [8]. In the Morse model the harmonic potential is replaced, in the Schrödinger equation (SE), by the the so-called Morse potential. This model can be solved analytically and reproduces faithfully the experimental vibrational levels of diatomic molecules, providing a spectrum with an upper bound. In order to obtain better fittings with the experimental data, several ab initio methods, based on the use of Morse-like, Kratzer-like or modified versions of these or other potential functions have been used to study molecular systems [9–12]. There are also several ab initio and algebraic methods to calculate dissociation energies [13,14].

Despite the fact that ab initio methods are able to obtain good approximations for spectra of many molecules, some authors have pointed out some limitations to these. Angelova et al. [15], noted that the Morse potential contains just quadratic corrections and one needs to use the empirical Dunham expansion to fit the highest vibrational energies. Iachello and Levine [16], remarked that the solution of the SE is very difficult in the case of two- and three-dimensions and, at this point, algebraic methods could bring some advantage. Problems related to the dissociation energy estimation and an algebraic energy method to calculate it, were described by Sun et al. [17]. Besides the facts above mentioned, there are some molecules whose potentials deviate strongly from Morse-like potentials [18].

The algebraic approach to study molecular vibrational and rotational spectra was pioneered by Iachello [19]. The method has been proved useful for accurately calculating highly excited vibrational levels and describing the whole spectrum of complex molecules, while maintaining its simplicity, in cases where the use of ab initio methods are not feasible in practice [20,21]. Furthermore, algebraic approach is able to provide the energy spectra of molecules without considering the shape of the potential and the Schrödinger equation. The method has been used to study the rotational and vibrational spectra of molecules [5,22]. A brief review of the Lie algebraic method in molecular and other systems can be seen in reference [23].

Deformed Heisenberg algebras (or q-oscillators) have attracted considerable attention since they have been proposed [24–26], due both to mathematical interest and

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to their possible physical applications [27] (see Ref. [28] for a review). They are non-trivial generalizations of the Heisenberg algebra having as generators ladder operators and the number operator. These algebras are characterized by the deformation parameter q. It is interesting to notice that for some set of values of the q-deformation parameter, namely $0 < q < 1$, the energy spectrum associated with the deformed Heisenberg algebras presents an upper bound, a situation which is similar to the typical spectrum of a composite particle [29]. This property suggests that deformed Heisenberg algebras might be a useful tool to investigate the spectrum of composite particles. Diatomic molecules are an important example of composite particles. Thus, deformed algebra approach has been used to study the molecular spectrum of diatomic molecules [15,30–32] as an alternative method to the usual ab initio approaches. Within this formalism q-oscillators are used as a model of anharmonic oscillators, whose spectrum is similar to the molecular vibrational spectrum. Advantages of this method are that it has few parameters, analytical expressions and fits well the first experimental levels. However, as it will become clear later, the model does not provide the correct dissociation energy for the CO molecule, for example, i.e., it fails to fit the highest vibrational levels.

Possible physical interpretations of the q-oscillator algebras, have been discussed in many works. For example, in molecular physics, the potential associated to the q-oscillator was studied by several authors [33–35]. In many-body theory, a possible interpretation of the q parameter was given by Sviratcheva et al. [36].

Recently, a generalized Heisenberg algebra (GHA), where the commutation relations among the operators depend on a characteristic function of the generalized number operator, has been proposed [26]. If the characteristic function is linear, with slope q^2, the algebra corresponds to the q-oscillator algebra. In the present work we introduce and implement a nonlinear GHA which is able to describe typical features of the vibrational molecular spectrum of the carbon monoxide molecule. The spectrum generated by this nonlinear GHA (nl-GHA) allows us to fit the 20 first vibrational transitions and to obtain the correct dissociation energy for the CO molecule, providing better global results than the methods above mentioned.

The paper is organized as follows. In Section 2 we discuss the solution of the Schrödinger equation (SE) with Morse potential. In Section 3 we introduce the GHA method. In Section 4 we apply our GHA model to the CO molecule. Finally, Section 5 is devoted to discussions and conclusions.

2 Morse potential for diatomic molecules: vibrational levels

Let us now turn our attention to one of the most familiar quantum description of diatomic molecules. For low energy levels, the molecular potential can be approximated by the harmonic potential, whereas for high energy levels this approximation breaks down. In fact, the higher vibrational transitions exhibits a certain degree of anharmonicity. Thus, to take into account anharmonic terms and rotational effects, nonlinear terms must be introduced in the energy expression besides the harmonic one [3]:

$$E_\nu = \sum_l = Y_{l,0}\left(\nu + \frac{1}{2}\right)^l, \tag{1}$$

where ν is the vibrational quantum number. The above expression corresponds to the expansion obtained by Dunhan, using the WKB method [1], without rotational terms. An analytical solution for the SE, which corresponds to the second order truncation of equation (1), was obtained by Morse [8] using the so-called Morse potential. The solution of the SE for this potential gives the following expression for the vibrational energy

$$\epsilon_n = -D + h\omega\left[\left(\nu + \frac{1}{2}\right) - \chi_e\left(\nu + \frac{1}{2}\right)^2\right],$$
$$(\nu = 0, 1, 2, ..., \frac{k-1}{2}), \tag{2}$$

where χ_e is a positive constant called the anharmonicity coefficient, ω is the fundamental frequency, ν is the vibrational quantum number and $k = 1/\chi_e > 1$. The anharmonicity coefficient is related to the dissociation energy:

$$\chi_e = \frac{h\omega}{4D}. \tag{3}$$

The energy levels obtained agree reasonably well with experimental data for many molecules [3]. The maximum allowed value for n in equation (2) is such that the SE solution remains finite. One can also show that this value is given by

$$\nu_{max} = \frac{1}{2\chi_e} - \frac{1}{2}. \tag{4}$$

Hence, there is a maximum energy value $\epsilon_{\nu_{max}}$ beyond which the system is not bounded.

In order to improve the Morse results, several perturbative methods, based on the Morse or other analytical or numerical potential, have been proposed. Huffaker [1], used a perturbed Morse model to calculate the first terms of the Dunhan expansion (1) for the CO molecule. He introduced a Morse-like potential function and using 28 spectral lines of the CO molecule [37], calculated eight parameters of the potential curve. This model is good when compared with the model obtained via RKR method by Mantz et al. [37]. If one ignores the rotational degree of freedom ($l = 0$), the model has seven parameters.

3 The generalized Heisenberg algebra

In [26], Curado e Rego-Monteiro proposed an algebra called GHA which is generated by three operators J_0, A and $A^\dagger$, which are generalizations of the usual number, creation annihilation operators, satisfying the following relations:

$$J_0 A^\dagger = A^\dagger f(J_0), \tag{5}$$

$$A J_0 = f(J_0) A, \tag{6}$$

$$\left[A, A^\dagger\right] = f(J_0) - J_0, \tag{7}$$

where † is the Hermitian conjugate, $(A^\dagger)^\dagger = A$, $J_0^\dagger = J_0$ and $f(J_0)$ is an analytical function of J_0, called the characteristic function. Assuming the existence of a vacuum state represented by $|0\rangle$ ($J_0|0\rangle \equiv \alpha_0|0\rangle$), it can be shown that

$$J_0 |m\rangle = f^m(\epsilon_0) |m\rangle, \quad m = 1, 2..., \tag{8}$$

$$A^\dagger |m\rangle = M_m |m+1\rangle, \tag{9}$$

$$A |m\rangle = M_{m-1} |m-1\rangle, \tag{10}$$

where $M_{m-1}^2 = f^m(\epsilon_0) - \epsilon_0$, ϵ_0 is the lowest J_0 eigenvalue and $f^m(\epsilon_0)$ is the mth iteration of the function f. This algebra describes a class of Heisenberg-like algebras of quantum systems, having J_0 eigenvalues given by

$$\epsilon_n = f(\epsilon_{n-1}), \tag{11}$$

where ϵ_n and ϵ_{n-1} are two successive eigenvalues [38]. Therefore, the J_0 eigenvalues can be obtained iteratively and they can be upper bounded or not, depending on the characteristic function, the values of the function parameters, and the initial value ϵ_0. For each kind of function, the values of the parameters and the initial values determine the existence or not of the fixed points, $\epsilon^\star = f(\epsilon^\star)$ [39], and their stability. As a consequence, different spectra are obtained for different functions and the eigenvalues behavior can be analyzed using dynamical systems techniques. For the linear case the characteristic function is $f(J_0) = q\,J_0 + s$, and the resulting algebra describes the one-parameter GHA studied in [26] and can be mapped into the q-oscillator algebra. If $q = 1$, the standard Heisenberg algebra is recovered. However, the connection between the generalized operators and the standard position and momentum operators is not known.

A graphical analysis of the functions $f(\epsilon) = q\epsilon + s$ and $y = \epsilon$ is shown in Figure 1. The intersection between the two lines is identified as the fixed point of the recurrence equation $\epsilon_n = q\epsilon_{n-1} + s$. The most interesting cases are obtained for $0 < q < 1$ and $\epsilon_0 < s/(1-q)$, as under these conditions the energy spectrum has an upper bound $\epsilon^* = s/(1-q)$.

This behavior is similar to the energy spectrum of bounded systems, for instance diatomic molecules, and $D_q \equiv \epsilon^* - \epsilon_0$ can be related to the dissociation energy of the system. This interesting result enables us to perform a phenomenological investigation of bounded systems, such as a diatomic molecule, via GHA. This approach has been performed by several authors [15,28].

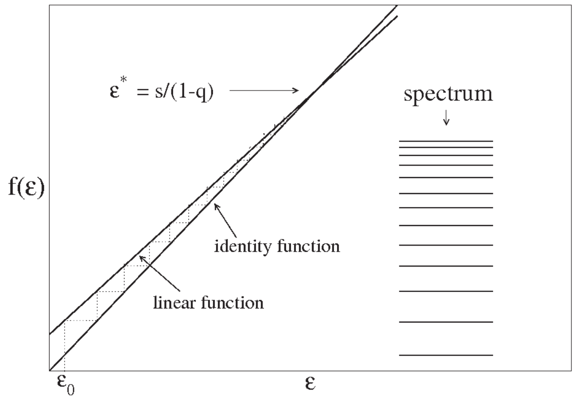

Fig. 1. Graphical analysis of a linear characteristic function, $f(\epsilon)$ for $0 < q < 1$ with $\epsilon_0 < s/(1-q)$. Note that, as the function is iterated, the energy value approaches the stable point $\epsilon^* = s/(1-q)$ (the upper bound). The dissociation energy of the system is proportional to $(\epsilon^* - \epsilon_0)$.

4 GHA and vibrational molecular spectrum

4.1 Linear case — (q-oscillator)

We will now study the spectrum generated by the linear GHA mentioned above, which correspond to the q-oscillator algebra. To study the vibrational spectrum of diatomic molecules via GHA formalism, we use a result developed in [39,40]. Let us start with the general Hamiltonian

$$H = \hbar\omega(c_1 A A^\dagger + c_2 A^\dagger A + c_3), \tag{12}$$

where A and $A^\dagger$ obey the relations (5–7) and c_1, c_2 and c_3 are real numbers. Choosing $c_1 = c_2 = 1$ and $c_3 = 0$, and using the equations (8-10) we get [39]

$$H = \hbar\omega\left(f(J_0) + J_0 - 2\epsilon_0\right). \tag{13}$$

Therefore, for the linear case $f(J_0) = qJ_0 + s$ ($q < 1$) we have:

$$H = \hbar\omega\left((q+1)J_0 + s - 2\epsilon_0\right). \tag{14}$$

We assume $s = 1$, once it does not affect the behaviour of the eigenvalues [26]. Applying the Hamiltonian (14) on the eigenstate $|\nu\rangle$ of J_0 (with $\hbar = 1$), we obtain $H|\nu\rangle = E_\nu|\nu\rangle$, where the energy eigenvalues are given by

$$E_\nu = \omega[(q+1)f^\nu(\epsilon_0) + s - 2\epsilon_0], \tag{15}$$

where $f^\nu(\epsilon_0) = q^\nu\epsilon_0 + s(q^\nu - 1)/(q-1)$. After some algebra we obtain

$$E_\nu = \omega\left(M_q - L_q q^{\nu+1/2}\right), \tag{16}$$

with

$$L_q = \frac{1+q}{q^{1/2}}\left(\epsilon_0 - \frac{s}{1-q}\right) = \frac{1+q}{q^{1/2}}(\epsilon_0 - \epsilon^*)$$

and

$$M_q = 2\left(\frac{s}{1-q} - \epsilon_0\right) = 2(\epsilon^* - \epsilon_0).$$

Table 1. Values of the parameters used in each model.

model	parameters	values
Morse	χ_e	0.0062
q-oscillator	q	0.98646
(linear GHA)	ϵ_0	36.98
nonlinear GHA	ϵ_0	0.9235
	q	0.9872
	p	-1.43×10^{-7}
perturbed Morse	σ	77.21317
(Huffaker)	τ	83769.28
	b_4	0.036067
	b_5	0.017505
	b_6	0.014945
	b_7	0.010770
	b_8	0.008142

The maximum energy ($\nu \to \infty$) for this system is given by $E_\infty = \omega M_q = 2\omega(\epsilon^* - \epsilon_0)$, and the dissociation energy ($E_\infty - E_0$) is then

$$D_q = \omega(1+q)(\epsilon^* - \epsilon_0). \tag{17}$$

The q-parameter can be interpreted as being related to the anharmonicity constant, $\chi_e = -\tau/2$, where $q = e^\tau$ [35].

We will now apply the above results to the carbon monoxide molecule spectrum and compare it with both experimental data and the spectra obtained by using the Morse, the perturbed Morse and the q-oscillator models. We used the data provided by the HITRAN database [41] and chose the lines in which the molecules are in the electronic fundamental state. Also, we selected the lines whose rotational quantum numbers are zero. Thus, there remained the spectral lines which represent the first 21 pure vibrational transitions of the CO molecule.

In order to fit the parameters (q and ϵ_0) to the experimental data, note that the logarithm of the difference between two successive levels of equation (16), as a function of ν, is a straight line with slope $\ln q$. Taking the logarithm of the difference between two successive data points, we obtain the value of q by evaluating the slope of the curve after a linear regression. The fitted parameters are shown in Table 1. The linear GHA spectrum agrees well with the experimental data (see Tab. 3 and Fig. 2) mainly in the case of the 20 first vibrational transitions. However, the D value calculated by equation (17) deviates strongly from the experimental value, as can be seen in Table 2. This means that, although the q-oscillator relative errors ($\Delta E = (E_{theor.} - E_{exp.})/E_{exp.}$) are smaller than the relatives error obtained by the Morse model, for most of the 20 first vibrational transitions (Fig. 2), the approach based on the q-oscillator is not able to fit higher frequency vibrational levels.

4.2 Nonlinear case

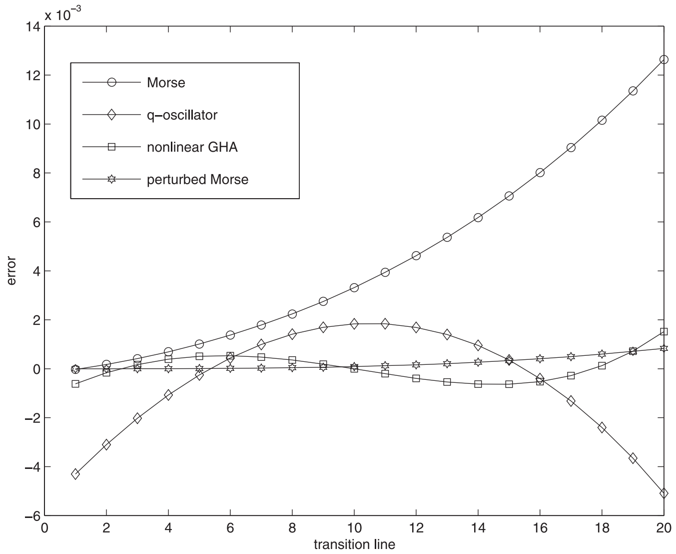

Fig. 2. Comparison between the relative errors of the Morse (○), q-oscillator (◇), nonlinear GHA (□) models and perturbed Morse ($\star$). We can see that the nonlinear GHA errors are smaller (in almost all data points) than the Morse and q-oscillator models.

Table 2. Values of the dissociation energy calculated for each model.

model	Dissociation energy (cm^{-1})
Experimental	89591.35
Morse	86426.44
q-oscillator	158970.48
Perturbed Morse (Ref. [1])	96476.01
Perturbed Morse (Ref. [14])	95394.23
nonlinear GHA	89987.76

As seen above, the linear GHA (i.e. the q-oscillator), is a good model only for the first levels. In order to fit the energy levels and to obtain the correct dissociation energy we were led to use a nonlinear functional $f(x)$ in GHA (5–7). We found that by using the functional

$$f(x) = p\,x^4 + q\,x + 1, \tag{18}$$

it is possible to obtain a good fit with the experimental data and the correct dissociation energy. Due to its nonlinearity, the spectrum generated by this nonlinear GHA does not have an analytical closed expression like equation (16). In this case the spectrum can only be calculated numerically.

For the sake of simplicity, we start from the Hamiltonian

$$H = \hbar w(A^\dagger A + \epsilon_0) = \hbar w J_0, \tag{19}$$

which is derived from Hamiltonian (12) with $c_1 = 0, c_2 = 1$ and $c_3 = \epsilon_0$. Replacing $f(J_0)$ given by equation (18) in relations (5–7) and applying H on the eigenstates of J_0 (with $\hbar = 1$) we obtain

$$E_\nu = w f^\nu(\epsilon_0), \tag{20}$$

where $f^\nu = \epsilon_\nu$ is given by:

$$\epsilon_{n+1} = p\epsilon_n^4 + q\epsilon_n + 1. \tag{21}$$

Table 3. Vibrational spectrum of the CO molecule. Comparison of the experimental data with the Morse, q-oscillator, perturbed Morse and GHA model. Botton: root mean square errors. Experimental data from HITRAN database. *There is a systematic difference of the 0.03 cm^{-1} between the data used in references [1,37].

	energy (cm^{-1})				
transition line	exp.	Morse	nonlinear GHA	linear GHA	perturbed Morse*
$1 \to 0$	2143.24	2143.30	2144.56	2152.46	2143.27
$2 \to 1$	2116.76	2116.39	2117.10	2123.32	2116.79
$3 \to 2$	2090.34	2089.48	2089.99	2094.57	2090.37
$4 \to 3$	2064.00	2062.57	2063.19	2066.21	2064.02
$5 \to 4$	2037.72	2035.66	2036.68	2038.23	2037.73
$6 \to 5$	2011.51	2008.75	2010.44	2010.63	2011.51
$7 \to 6$	1985.38	1981.84	1984.43	1983.41	1985.35
$8 \to 7$	1959.32	1954.93	1958.62	1956.55	1959.26
$9 \to 8$	1933.33	1928.01	1932.97	1930.06	1933.24
$10 \to 9$	1907.43	1901.10	1907.43	1903.93	1907.29
$11 \to 10$	1881.61	1874.19	1881.99	1878.15	1881.40
$12 \to 11$	1855.85	1847.28	1856.58	1852.72	1855.59
$13 \to 12$	1830.19	1820.37	1831.18	1827.63	1829.84
$14 \to 13$	1804.61	1793.46	1805.74	1802.89	1804.16
$15 \to 14$	1779.11	1766.55	1780.23	1778.48	1778.55
$16 \to 15$	1753.69	1739.64	1754.61	1754.39	1753.00
$17 \to 16$	1728.36	1712.73	1728.85	1730.64	1727.53
$18 \to 17$	1703.12	1685.82	1702.90	1707.21	1702.13
$19 \to 18$	1677.96	1658.91	1676.75	1684.09	1676.79
$20 \to 19$	1652.88	1632.00	1650.37	1661.29	1651.53
rms error	-	0.0013	0.00048	0.00012	0.00007

We use the values generated by equation (20) with $f^{\nu}(\epsilon_0)$ given by equation (21) in order to fit the q, p and ϵ_0 parameters with the experimental data. The dissociation energy is given by

$$D_{GHA} = E_{\infty} - E_0 = w(\epsilon^* - \epsilon_0), \tag{22}$$

where ϵ^* is the stable fixed point of the recurrence equation (21).

The fitted parameters are shown in Table 1. The dissociation energy is shown in Table 2. In Table 3 we compare the energy levels obtained with the different models referred in this work with the experimental data. The relative errors are shown in Figure 2. We can see that the nonlinear GHA with the functional 18 provides better fittings with experimental data than both the q-oscillator and Morse models and it is comparable to the Huffaker model [1]. Furthermore, nonlinear GHA provides a more accurate dissociation energy when compared to that obtained in all other methods. These results show that our model is a good method for obtaining the higher anharmonic energy levels of the CO molecule.

As the p parameter is very small (Tab. 1), if ϵ_0 is also small, the first iterations of equation (21) are dominated by the linear term. The nonlinear term becomes relevant as the number of iterations increase. The difference between two successive energy levels decreases up to zero as the function (21) is iterated. Because the p parameter is negative, the difference between two successive energy levels tends to zero. Thus, the nonlinear term flattens the energy curve faster than in the pure linear and the perturbed Morse cases, but slightly slower than the Morse Model, as we can see in Figure 3.

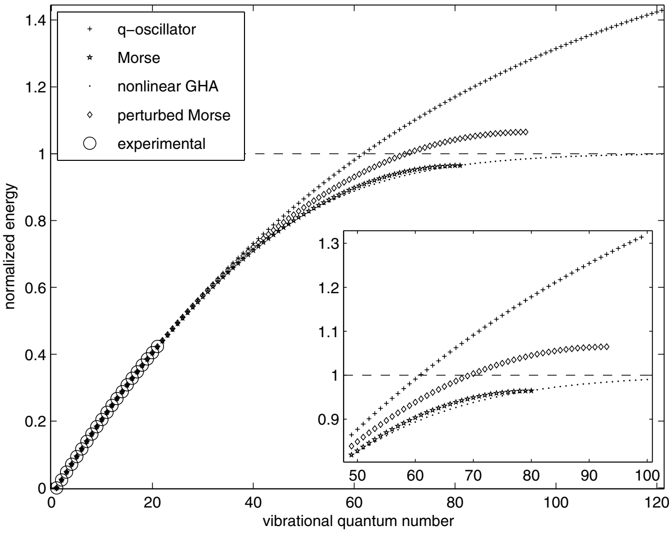

Fig. 3. Normalized and shifted energy spectrum generated by the Morse ($\star$), q-oscillator ($+$), perturbed Morse ($\diamond$) and nonlinear GHA ($\cdot$) models, and experimental data ($\circ$). The dashed line represents the normalized experimental dissociation energy value. We can see that the dissociation energy of the nonlinear GHA lies on the experimental dissociation energy (dashed curve) while the q-oscillator and Morse spectrum are respectively above and below dissociation energy line. Inset figure shows in detail the Morse and the nonlinear GHA energy curves close to dissociation energy line. Note that the Morse curve flattens before reaching the experimental dissociation energy while the nonlinear GHA energy curve approach it as ν increase.

We would like to stress that besides these accurate fittings, the nonlinear GHA give us an extremely simple way to estimate higher transitions of CO. We only need to iterate equation (21) up to the required level.

5 Conclusion and perspectives

In this work we have proposed a method based on GHA to reproduce the vibrational molecular spectrum of diatomic molecules. For the CO molecule, we have shown that the previous method based on the q-oscillator algebra (linear GHA) reproduce the vibrational molecular spectrum for the 20 first vibrational transitions of the CO molecule, but it does not provide the correct dissociation energy, i.e., this model fails when describing higher vibrational levels. Using a nonlinear functional (4th order) in the GHA we were able to fit the experimental energy levels and to calculate the dissociation energy for the CO molecule with good accuracy. For this molecule the nonlinear GHA has provided better global results than the usual Morse and perturbed Morse models, and the q-oscillator model. This work shows that GHA can be used as a simple phenomenological tool to study composite particles.

GHA produces different spectra for different characteristic functions. The GHA spectrum could be related to deformations in the harmonic potential. Indeed, this algebra can reproduces a variety of spectra once we are able to find the appropriate characteristic function. Consequently, this algebra could be used to study other molecules, by simply choosing the appropriate characteristic function. In an even more general fashion, de Souza et al. [42] have constructed a more general structure that depends on two functional. This new algebraic structure can reproduce a even greater variety of the spectrum behaviour, allowing us to work with two quantum numbers.

We have introduced a new method which is a generalization of former algebraic methods. The method was tested for the CO molecule and was able to fit accurately the experimental data of the 20 first transitions, to predict unknown levels, and to calculate the correct dissociation energy. The results obtained in this work motivate us to explore deeper the relation between the GHA and molecular systems. These investigations may include: (1) the study of the relation between the functional parameters and the molecular parameters; (2) the investigation of the potential curve underlying the GHA; (3) the account of electronic and rotational states; (4) the study of the applicability of the GHA method for larger molecules. Items 3 and 4 could be performed by choosing other characteristic functions and/or extending the number of operators.

We thank E.M.F. Curado and M.A. Rego-Monteiro for fruitful discussions and remarks and S. Queiros, N. Lemke, E.R.P. Delfin, F.D. Nobre and F. Baldovin for manuscript revision. We thank the referees for their careful reading of the manuscript, constructive comments and suggestions. We would also like to acknowledge the partial support of CNPq and PRONEX (Brazilian agencies).

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