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# Calculation of Energy Eigenvalues and Wave Functions of the Deng-Fan Oscillator

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**Abstract:** Determination of the analytical expressions for the energy eigenvalues and the corresponding wave functions of the quantum anharmonic oscillator with a Deng-Fan potential, using an approach, based on the Floquet theorem and the resonating averages method. The obtained analytical results are applied to H<sub>2</sub>, O<sub>2</sub> and HF diatomic molecules. The Comparison of our results agrees well, with those available in the literature.

## 1 INTRODUCTION

The study of quantum anharmonic oscillator plays a role of great interest in several fields of physics and chemistry. Notably, it is one of the physical systems which allows the description of the energies of vibration and rotation of the diatomic molecules. On this topic, there are several empirical functions of anharmonic oscillator that have been implemented to describe the energy spectra of diatomic molecules and electromagnetic transitions [1] [2]. Among the well-known potential functions in the literature have been proposed by Morse it is the most model used in the investigation of diatomic molecules [2] [3] [4]. Thus, numerous studies have been devoted to improving the form of the Morse potential function in order to obtain an accurate numerical calculation, of the energy eigenvalues and wave functions, in good agreement with the experimental results. In particular, we cite the work of Deng and Fan who proposed to modify the form of the Morse potential [1] [2]. This new form called the Deng-Fan oscillator or also the generalized Morse potential [1] [2]. In this regard, many procedures and methods was been explored and applied to calculate the eigenvalue of the energy of this system.

Our motivation in this work is based on the exploitation of the results, learned from our previous papers [5] [6], for the Deng-Fan oscillator which is developed up to order four. The elaboration of our

analytical results was carried out using Floquet's theorem and the resonating averages method.

The structure of our communication is as follows, in section 2, we give the main equations and we deduce the analytical expressions of the wave functions and the second order vibrational energies. In section 3, we apply these expressions to some diatomic molecules (H<sub>2</sub>, O<sub>2</sub> and HF) and we compare our results with those published in the literature obtained from other methods [7] [8]. Section 4 contains the conclusions.

## 2 BASIC EQUATIONS

The Deng-Fan potential is given by [1] [2]

$$V(q) = D \frac{(1 - e^{-\rho q})^2}{(1 - e^{-\rho(q+r_e)})^2} \quad (1)$$

Where D is the dissociation energy,  $\rho$  is the scaling factor of the Morse potential,  $r_e$  is the equilibrium internuclear distance and q is the variation of interatomic distance with respect to the equilibrium distance.

The Taylor development of V(q) to the fourth order around q gives:

$$V(q) = \frac{D\rho^2}{(\alpha-1)^2} q^2 + \frac{D\rho^3}{(\alpha-1)^3} (1+\alpha) q^3 + \frac{1}{12} \frac{D\rho^4}{(\alpha-1)^4} (7\alpha^2 + 22\alpha + 7) q^4 \quad (2)$$

where

$$\alpha = e^{-\rho r_e} \quad (3)$$

The Hamiltonian of the Deng-Fan oscillator can be written as,

$$H = \frac{p^2}{2m} + \frac{D\rho^2}{(\alpha-1)^2} q^2 + \frac{D\rho^3}{(\alpha-1)^3} (1+\alpha) q^3 + \frac{1}{12} \frac{D\rho^4}{(\alpha-1)^4} (7\alpha^2 + 22\alpha + 7) q^4 \quad (4)$$

The expression of this Hamiltonian is comparable to that given by equation (5) of the reference [6]. Then, we make the change of the following coefficients

$$\omega_0 = \frac{\rho}{(\alpha-1)} \sqrt{\frac{2D}{m}} \quad (5a)$$

$$\mu_1 = -\frac{D\rho^3(\alpha+1)}{\hbar\omega_0(\alpha-1)^3} \left( \frac{\hbar}{m\omega_0} \right)^{\frac{3}{2}} \quad (5b)$$

$$\mu_2 = -\frac{D\rho^4(7\alpha^2 + 22\alpha + 7)}{12\hbar\omega_0(\alpha-1)^4} \left( \frac{\hbar}{m\omega_0} \right)^2 \quad (5c)$$

Using Eq. (24) and Eq. (35) of our paper [5], we obtain the quasi-energy  $^{(2a)}E_n$  up to the second ameliorated order such as,

$$\begin{aligned} ^{(2a)}E_n = & \hbar\omega_0 \left[ \frac{1}{8} \left( 3\mu_2 - \frac{7}{2}\mu_1^2 \right) + \left( 1 - \frac{67}{16}\mu_2^2 \right) \left( n + \frac{1}{2} \right) - \frac{3}{4} (5\mu_1^2 - 2\mu_2) \left( n + \frac{1}{2} \right)^2 \right. \\ & \left. - \frac{17}{4}\mu_2^2 \left( n + \frac{1}{2} \right)^3 \right] \end{aligned} \quad (6)$$

By using the Eq. (10) of [6], we determine the second-order wave functions as follows,

$$^{(2a)}\psi_n(\hat{q}) = \left( \frac{m\omega_0}{\hbar\pi} \right)^{\frac{1}{4}} \frac{e^{-\frac{\hat{q}^2}{2}}}{\sqrt{2^n n!}} \sum_{j=0}^{n+8} C_{n+j}^n H_{n+j}(\hat{q}) \quad (7)$$

where  $H_n(\hat{q})$  are the Hermite polynomials.

The coefficients  $C_{n+j}^n$  of the Eq. (6) are given by

$$C_{n-8}^n = \frac{\mu_2^2}{32} \frac{n!}{(n-8)!} \quad (8)$$

$$C_{n-7}^n = \frac{\sqrt{2}}{192} \mu_1 \mu_2 \frac{n!}{(n-7)!} \quad (9)$$

$$C_{n-6}^n = \frac{1}{2} \left[ \frac{\mu_1^2}{9} + \left( n - \frac{11}{6} \right) \frac{\mu_2^2}{2} \right] \frac{n!}{(n-6)!} \quad (10)$$

$$C_{n-5}^n = \frac{17}{24} \mu_1 \mu_2 \left( n - \frac{104}{85} \right) \frac{n!}{(n-5)!} \quad (11)$$

$$C_{n-4}^n = \frac{1}{4} \left[ \mu_2 + \left( 2n - \frac{3}{2} \right) \mu_1^2 + (n-1) (2n-7) \mu_2^2 \right] \frac{n!}{(n-4)!} \quad (12)$$

$$C_{n-3}^n = \left[ \frac{\mu_1}{3} + (21n^2 - 74n + 29) \frac{\mu_1 \mu_2}{16} \right] \frac{n!}{(n-3)!} \quad (13)$$

$$\begin{aligned} C_{n-2}^n = & \frac{1}{2} \left[ (2n-1) \mu_2 + (7n^2 - 19n + 1) \frac{\mu_1^2}{4} - (4n^3 + 60n^2 - 16n + 15) \frac{\mu_2^2}{8} \right] n(n-1) \end{aligned} \quad (14)$$

$$\begin{aligned} C_{n-1}^n = & \frac{1}{2} \left[ 3n\mu_1 - (81n^3 + 834n^2 + 203n + 274) \frac{\mu_1 \mu_2}{48} \right] n \end{aligned} \quad (15)$$

$$C_n^n = 1 + \frac{\mu_1^2}{144}(2n+1)(82n^2 + 82n + 87) + \frac{1}{256}\mu_2^2(65n^4 + 130n^3 + 487n^2 + 422n + 156) \quad (16)$$

$$C_{n+1}^n = \frac{1}{4} - 3(n+1)\mu_1 + (-81n^3 + 591n^2 + 1222n + 816)\frac{\mu_1\mu_2}{48} \quad (17)$$

$$C_{n+2}^n = \frac{1}{8}[-(2n+3)\mu_2 + (7n^2 + 33n + 27)\frac{\mu_1^2}{4} + (4n^3 + 48n^2 + 142n + 87)\frac{\mu_2^2}{8}] \quad (18)$$

$$C_{n+3}^n = \frac{1}{8}\left[-\frac{\mu_1}{3} + (21n^2 + 116n + 124)\frac{\mu_1\mu_2}{16}\right] \quad (19)$$

$$C_{n+4}^n = \frac{1}{64}\left[-\mu_2 + \left(2n + \frac{7}{2}\right)\mu_1^2 + (2n^2 + 13n + 13)\mu_2^2\right] \quad (20)$$

$$C_{n+5}^n = \frac{17}{768}\left(n + \frac{108}{85}\right)\mu_1\mu_2 \quad (21)$$

$$C_{n+6}^n = \frac{1}{128}\left[\frac{\mu_1^2}{9} + \left(n + \frac{17}{6}\right)\frac{\mu_2^2}{2}\right] \quad (22)$$

$$C_{n+7}^n = \frac{\mu_1\mu_2}{1536} \quad (23)$$

$$C_{n+8}^n = \frac{\mu_2^2}{8192} \quad (24)$$

Where the coefficients  $\mu_1$  and  $\mu_2$  are given by equations (5), and which are the amplitudes of the cubic and quadratic perturbation respectively.

### 3 NUMERICAL RESULTS

To illustrate the analytical results given by equations (6) and (7), we represent the wave function and the corresponding probability density for the numerical values of the  $H_2$  molecule, and we determine the vibrational energy values of the  $H_2$ ,  $O_2$  and  $HF$  molecules for the first five values of the quantum number  $n$ .

To adjust the units of physical quantities we used the following conversion, throughout our numerical computation,

$$m \times 10^{-23} g = m \times 6.02214 \times 931.494 \times 10^6 eV / c^2$$

with  $\hbar c = 1973.29 eV \text{ \AA}$ .

Table 1 indicate that the comparisons of our numerical values of vibrational energies for  $H_2$ ,  $O_2$  and  $HF$  molecules with those of the authors, Oyewumi and Sen [8] and Falaye et al. [7], presents few differences. This is due to the restriction made in the Taylor expansion series of  $V(q)$ . Because we truncated the potential expansion of Deng-Fan only to the fourth order.

Figure 1 and Figure 2 show that the graphs of the wave functions and the corresponding probability densities retain their nodal aspect. However, they present the asymmetrical form this is due to the anharmonic effect of the Deng-Fan potential.

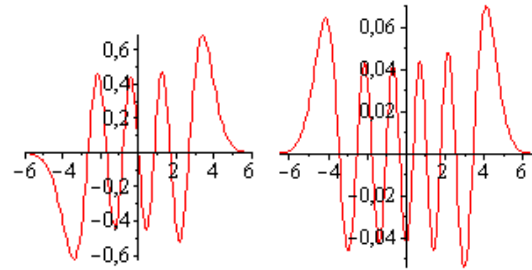


Figure 1: The wave function vs.  $\hat{q}$  for  $n=7$  and  $n=10$ .

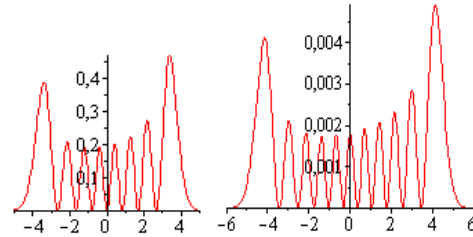


Figure 2: The probability density vs.  $\hat{q}$  for  $n=7$  and  $n=10$ .

Table 1 : Numerical values of vibrational energies (in eV) of H<sub>2</sub>, O<sub>2</sub> and HF diatomic molecules for n=0 to n=4.

n	Our study (H <sub>2</sub> )	Literature (H <sub>2</sub> )[8]	Our study (O <sub>2</sub> )	Literature (O <sub>2</sub> )[7]	Our study (HF)	Literature (HF)[7]
0	0.3618	0.38021	0.1026	0.1020	0.2781	0.2966
1	1.1267	1.1368	0.3108	0.3015	0.8531	0.8487
2	1.9185	1.8935	0.5229	0.4974	1.4492	1.3747
3	2.7089	2.6502	0.7386	0.6891	2.0629	1.8697
4	3.4696	3.4068	0.9577	0.8767	2.6907	2.3344

Table 2: Parameters of the selected molecules [7].

Molecules	D (cm <sup>-1</sup> )	$\rho(^{\circ}A^{-1})$	$r_e(^{\circ}A)$	m (10 <sup>-23</sup> g)
H <sub>2</sub>	38318	1.9506	0.741	0.084
O <sub>2</sub>	42041	2.6636	1.207	1.337
HF	49382	2.2266	0.917	0.160

## 4 CONCLUSIONS

We have used our previous analytical results of the references [5] [6], obtained by applying the method of Floquet theorem combined with the resonating averages method, in order to obtain the approximate solutions of the Schrodinger equation of the Deng-Fan oscillator whose potential is developed to four order. The vibrational energies and the wave functions for this molecular potential are obtained up to the second order correction.

To illustrate the analytical expressions established for the wave functions and the vibrational energy levels we have used the parameters of the H<sub>2</sub>, O<sub>2</sub> and HF diatomic molecules. In Figure 1 and Figure 2 we have plotted the curves of the wave functions as well as the probability density, which shows that they have the regular nodal character and they are not symmetrical, they are not symmetrical because of the anharmonic effect of Deng- Fan potential. In addition, the calculation of the numerical values of the vibrational energy levels, carried out for the H<sub>2</sub>, O<sub>2</sub> and HF molecules are presented in table 1, these show that our numerical results agree with to those published by the authors Oyewumi, Sen [8] and Falaye et al. [7]. In future work, we plan to apply our

approach where the Deng-Fan potential will be developed by a Taylor series of high order.

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