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Quantum Anharmonic Oscillator, A Computational Approach

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Abstract

What is *anharmonicity*?

What happens to the *energy levels* of an anharmonic oscillator?

What is *dissociation energy*?

Many such questions can be answered by the computational method. The ***computational methods*** used for solving the second degree differential equation (Schroedinger's equation) is **by Runge-Kutta fourth order method** using **Microsoft-Excel**.

For anharmonic oscillator, the accuracy of the results is fairly good.

***The computation and animation will be sent along this for publication/ online view**

I. INTRODUCTION

For anharmonic oscillator [1],[2], the potential is given by

$$V = \tfrac{1}{2}kx^2 + bx^4 \quad \text{where } b \text{ is a constant.} \tag{1}$$

as shown in Fig. 1

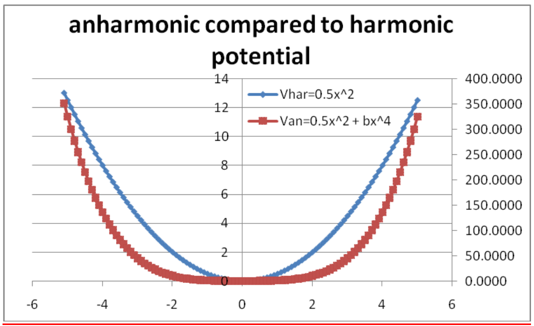

Fig. 1 Anharmonic Potential (darker brown) with b = 0.5

II. THEORY

When Eq. 1 is used in the Schroedinger's equation, the allowed vibrational energy levels [3] is found to be

$$E_{an} = (n+\tfrac{1}{2}) - \tfrac{3}{2}b(n^2+n+\tfrac{1}{2}) + \tfrac{b^2}{8}(34n^3+51n^2+59n+21) \tag{2}$$

$$\text{where } n = 0,1,2,\ldots$$

Thus, the anharmonic oscillator behaves like the harmonic oscillator but with an oscillation frequency that decreases steadily with increasing *n*.

For the ground state ($n = 0$) we have

$$E_{0an} = 0.5 - 1.5b*0.5 + 0.125b^2 * 21 \tag{3}$$

The energy difference between consecutive levels decreases successively. Finally, when the energy difference is zero, the corresponding potential energy is a measure of the ***dissociation energy*** of the molecule.

III. METHODOLOGY

The computational output is obtained using **Microsoft Excel** .**Runge Kutta Fourth Order** is used for solving the Schroedinger's second degree ordinary differential equation. Of course, animation is done using **graphics.**

IV. RESULT

- The energy is lesser than the harmonic oscillator [4] given by

$$\Delta E = \frac{3}{2}b(n^2 + n + \frac{1}{2}) - \frac{b^2}{8}(34n^3 + 51n^2 + 59n + 21) \tag{4}$$

The energy difference decreases with the increase of the quantum number *n* as shown below. On the other hand, the energy difference remains a constant for a harmonic oscillator.

Table 1. Comparison of energy in Anharmonic (Ean) and Harmonic Oscillators (Ehar)

		For b=	0.001
n	**Ean**	**ΔEan=En+1-En**	**Ehar**
0	0.499		0.5
1	1.496	0.997	1.5
2	2.490	0.994	2.5
3	3.481	0.991	3.5
4	4.469	0.988	4.5
5	5.454	0.985	5.5
6	6.435	0.982	6.5
7	7.413	0.978	7.5
8	8.389	0.975	8.5
9	9.361	0.972	9.5
..	..		
100	81.035		100.5
101	81.602	0.567	101.5
..	..		
150	102.036		150.5
151	102.292	0.256	151.5

..	..		
175	106.325		175.5
176	106.402	0.077	176.5
..	..		
185	106.755		185.5
186	**106.756**	0.001	186.5
187	106.749	-0.007	187.5

- The ***dissociation energy*** is ~ 106.756 units [5].

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