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Ground State Energy Eigenvalues of an Octic Oscillator with Quartic and Sextic Anharmonicities

Gayathri G. M.[1], B. A. Kagali[2], T. Shivalingaswamy[3]

[1]Department of Physics, HKES(SVP)College,Bangalore-560081, India.
[2]Department of Physics, Bangalore University, Bangalore-560056, India
[3]Corresponding Author: Department of Physics, Government College (Autonomous), Mandya-571401, India

Abstract: ***Here we derive the energy eigenvalues of an octic anhormonic oscillator that also has quartic and sextic anharmonic terms using Ginsberg-Montroll method. Numerical values are computed using Mathematica for different values of the anharmonic coefficients.***

Keywords: Quantum anharmonic oscillators; Ginsberg-Montroll method; Approximation Methods; Energy eigenvalues; Mathematica

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1. Introduction

Quantum mechanical anhormonic oscillators(AHO) have been studied by various methods. They are found to play an important role in various fields such as Molecular Physics, Solid state physics, field theory, Laser optics etc. Since perturbation theory breaks down, a variety of non-perturbative approximation methods have been employed to study them. Some of the methods are WKB approximation [1, 2], Hill determinant method [3], action-angle technique [4], Continued fraction method [5], the variational method [6, 7], Re-normalised frequency method [8] Chebyshev polynomial method [9], the residue-squaring method [10], Pade approximants method [11], the kinetic potential method [12], the fixed point method [13], the hypervirial method [14] and so on. One of the simplest methods was proposed by Ginsberg and Montroll [15].

2. Ginsberg-Montroll Method

In this method, the asymptotically correct wavefunction for the chosen anharmonic oscillator is first determined. Then, an interpolative wavefunction that has the same asymptotic behaviour but with several free parameters is assumed. The free parameters are fixed by solving the Schrödinger equation for the anharmonic oscillator. The energy eigenvalues are obtained by solving a polynomial equation that arises from the requirement of self consistency on the free parameters. We now apply the method to an octic oscillator that contain both quartic and sextic anharmonic terms. Such a situation is more realistic than the case of pure octic oscillators [16].

The Schrödinger equation for a one dimensional octic oscillator with quartic and sextic terms can be written as

$$\left\{-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{1}{2}Kx^2+\mu' x^4+\eta' x^6+\lambda' x^8-E\right\}\psi(x)=0 \quad (1)$$

By changing the variable to

$$y=\left(\frac{m\omega}{\hbar}\right)^{\frac{1}{2}}x,$$

and putting

$$\omega^2=\frac{K}{m},\ \varepsilon=\frac{E}{\hbar\omega},\ \mu=\frac{2\mu'\hbar}{m^2\omega^3},\ \eta=\frac{2\eta'\hbar^2}{m^3\omega^4},\ \lambda=\frac{2\hbar^3\lambda'}{m^4\omega^5},$$

we get the dimensionless equation:

$$\left(\frac{1}{2}\frac{d^2}{dy^2}-\frac{1}{2}y^2-\mu y^4-\eta y^6-\lambda y^8+\varepsilon\right)\psi(y)=0 \quad (2)$$

For large $|y|$, we obtain the asymptotic solution

$$\psi^{(8)}(y)\sim\exp\left\{-\frac{\sqrt{2\lambda}}{5}y^5\right\} \quad (3)$$

Hence $b_4=\frac{2\lambda}{25}$.

For the full wavefunction we postulate the following:

$$\psi^{(8)}=\text{const.}\left\{\exp\left\{-\left(b_1y^4+b_2y^6+b_3y^8+b_4y^{10}\right)^{\frac{1}{2}}\right\}\right\} \quad (4)$$

This reduces to the correct form in the case of a pure harmonic oscillator.

The coefficients b_1, b_2 and b_3 are determined by solving the equation (2) with the wave function of equation (4).

For small $|y|$, we expand the exponential in a power series and write

$$\psi^{(8)};\text{const.}\left\{\exp\left\{-\left(d_2y^2+d_4y^4+d_6y^6+d_8y^8+.....\right)\right\}\right\} \quad (5)$$

where

$$d_2=b_1^{\frac{1}{2}},\ d_4=\frac{1}{2}b_2b_1^{-\frac{1}{2}},\ d_6=b_1^{\frac{1}{2}}\left\{\frac{1}{2}\frac{b_3}{b_1}-\frac{1}{8}\left(\frac{b_2}{b_1}\right)^2\right\} \quad (6)$$

$$d_8=b_1^{\frac{1}{2}}\left\{\frac{1}{2}\frac{b_4}{b_1}-\frac{1}{4}\frac{b_2b_3}{b_1^2}+\frac{1}{16}\left(\frac{b_2}{b_1}\right)^3\right\}$$

Substituting this wavefunction into equation (2) and equating the coefficients of y^0, y^2, y^4 and y^6 to zero, we get the following set of equations for the original parameters b_1, b_2 and b_3:

$$b_1^{\frac{1}{2}}-\varepsilon=0 \quad (7)$$

$$-6b_2b_1^{\frac{1}{2}}+4b_1^2-b_1=0 \quad (8)$$

$$-30b_1^{\frac{1}{2}}\left\{\frac{1}{2}\frac{b_3}{b_1}-\frac{1}{8}\left(\frac{b_2}{b_1}\right)^2\right\}+8b_2-\mu=0 \quad (9)$$

and $$-56b_1^{\frac{1}{2}}\left\{\frac{1}{2}\frac{b_4}{b_1}-\frac{1}{4}\frac{b_2b_3}{b_1^2}+\frac{1}{16}\left(\frac{b_2}{b_1}\right)^3\right\}+b_1\left\{\frac{12b_3}{b_1}+\frac{b_2^2}{b_1^2}\right\}-\eta=0 \quad (10)$$

By eliminating b_1, b_2 and b_3 and using $b_4=\frac{2\lambda}{25}$ we get the following polynomial equation for ε:

$$94800\varepsilon^5-36600\varepsilon^3-3225\varepsilon-14400\mu\varepsilon^2+1575\mu+10125\eta-22680\lambda=0 \quad (11)$$

We can get the ground state energy eigenvalues by solving equation (11) for different values of anharmonic coefficients.

3. The Energy eigenvalues

For a pure octic oscillator $(\mu=0,\eta=0)$ we get the results as tabulated in Table 1 for ε, the exact values are also listed therein, for comparison[17].

Table 1: The ground state Energy eigenvalues $\varepsilon\left(\frac{E}{\hbar\omega}\right)$ of a pure octic oscillator

λ	ε(Our method)	ε(Exact values)
.000	0.50000	0.50000
.010	0.530199	0.53210
.100	0.629406	0.62051
.000	0.852045	0.82069
.00	1.25496	1.1909
.0	1.92777	1.8163
.0	3.01645	2.8331

These energy eigenvalues agree exactly with those obtained by us earlier[18].

For very large values of λ, we get

$$\varepsilon;0.75\lambda^{\frac{1}{5}}$$

in agreement with the calculations reported earlier[19]. The following tables list the values of ε for selected anharmonic coefficients (calculated using Mathematica [20]).

Table 2: The ground state Energy eigenvalues $\varepsilon\left(\frac{E}{\hbar\omega}\right)$ of a octic oscillator with equal sextic and quartic anharmonicities

λ	$\varepsilon(\text{for } \mu=\eta=0.01)$	$\varepsilon(\text{for } \mu=\eta=0.1)$	$\varepsilon(\text{for } \mu=\eta=1.0)$	$\varepsilon(\text{for } \mu=\eta=10)$
.000	0.51866	0.59881	0.825089	1.3585
.010	0.542001	0.608117	0.826901	1.35872
.100	0.633522	0.666091	0.842281	1.3607
.000	0.85314	0.862828	0.946884	1.37972
.00	1.25527	1.25806	1.28546	1.5197
.0	1.92787	1.92878	1.93786	2.02692
.0	3.01648	3.01681	3.0201	3.05287

Table 3: The ground state Energy eigenvalues $\varepsilon\left(\frac{E}{\hbar\omega}\right)$ of a octic oscillator with unequal sextic and quartic anharmonicities

λ	$\varepsilon(\mu=0.01,\eta=1.0)$	$\varepsilon(\mu=0.1,\eta=1.0)$	$\varepsilon(\eta=0.01,\mu=1.0)$	$\varepsilon(\eta=0.1,\mu=1.0)$
.000	0.757639	0.763895	0.698726	0.718061
.010	0.759979	0.766183	0.703917	0.722366
.100	0.77953	0.785326	0.741371	0.754644
.000	0.903113	0.907114	0.903332	0.907759
.00	1.26506	1.26692	1.27602	1.27689
.0	1.9295	1.93026	1.93625	1.93639
.0	3.01675	3.01705	3.01983	3.01986

4. Results and Discussions

It can be seen that Ginsberg-Montroll method works very well for small values of the anharmonic coefficients. This is to be expected since the wavefunction is obtained by solving the Schrödinger equation near the origin, while the anharmonic potential becomes significant away from the origin for large anharmonicities. Further, as we have used the wavefunction that corresponds to octic oscillator, the eigenvalues are exactly as that of pure octic oscillator when other anharmonicities are removed. It would be very interesting if we can choose a wave function which is a superposition of different anharmonic oscillators with suitable weight factors, this may help us to see that the eigenvalues reduce to different pure anharmonic oscillators whenever only the corresponding anharmonic coefficients are chosen. We have taken up the matter for further investigation.

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