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Ground States of Sextic and Octic Anharmonic Oscillators

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ABSTRACT

The ground state energy eigenvalues and eigenfunctions of sextic and octic anharmonic oscillators are obtained using the method of Ginsberg and Montroll. The numerical values thus obtained for various anharmonicities are compared with those derived from other methods. It is remarkable that the results obtained from this rather simple method agree within a few percent of exact values derived by lengthy calculations.
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Introduction

Quantum anharmonic oscillators have been studied by variety of methods [1,2]. One of the simpler methods is the one proposed by Ginsberg and Montroll [3]. Theirs is an interpolative perturbative scheme which has been shown to yield fairly accurate results for quartic anharmonic oscillators. In this article, we apply their method to sextic and octic oscillators. We find that this method can yield eigenvalues within few percent of the exact values [4]. Better agreement is found for smaller anharmonic parameters, in contrast with the method recently proposed by us [5], where better agreement with the exact values is obtainable for larger anharmonic parameters.

The Method

In the method of Ginsberg and Montroll [3] wave functions with proper asymptotic behaviour are chosen. The parameters of the wave function are determined by solving the Schrödinger equation near the origin. The energies are found by solving polynomial equations that result from requirements of self-consistency.

A) The Sextic Oscillator : The Schrödinger equation for a one dimensional sextic oscillator is

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

By changing the variable to $y = x\left(\frac{m\omega}{\hbar}\right)^{\frac{1}{2}}$ and with $\lambda=\frac{\lambda'\hbar^2}{m^3\omega^4}$, $\varepsilon=\frac{E}{\hbar\omega}$, $\omega^2=\frac{K}{m}$, the equation (1) becomes

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

For large $|y|$, $\psi(y)\sim\exp\left[-\sqrt{\frac{\lambda}{8}}\,y^4\right]$ .....(3)

and for small $|y|$, $\psi(y)\sim\exp[-\beta y^2]$ ..... (4)

Hence, we postulate the following interpolative function for the ground state

$$\psi_0^{(6)}(y)=\text{constant}\times\exp\left[-(a_1y^4+a_2y^6+a_3y^8)^{\frac{1}{2}}\right] \quad \text{.....(5)}$$

Near the origin, we can write

$$\psi_0^{(6)}(y)=\text{constant}\times\exp[-(c_2y^2+c_4y^4+c_6y^6+\ldots\ldots)] \quad \text{.....(6)}$$

where

$$c_2=a_1^{1/2},\ c_4=\frac{1}{2}a_2a_1^{-1/2},\ c_6=\frac{\lambda}{16}a_1^{-1/2}-\frac{1}{8}a_2^2a_1^{-3/2},\ldots\ldots \quad \text{.....(7)}$$

Therefore,

$$\frac{1}{2}\frac{d^2}{dy^2}\psi_0^{(6)}=[-c_2+2(c_2^2-3c_4)y^2-(15c_6-8c_2c_4)y^4+\ldots\ldots]\psi_0^{(6)} \quad \text{.....(8)}$$

Substituting (8) and (6) into Schrödinger equation and setting the coefficients of $y^0, y^2 y^0, y^2$ and $y^4 y^4$ to zero, we obtain

$$a_1^{1/2}-\varepsilon=0$$

$$-3a_2a_1^{-1/2}+2a_1-\frac{1}{2}=0 \quad \text{.....(9)}$$

$$4a_2-\frac{15}{2}a_1^{1/2}\left\{\frac{a_3}{a_1}-\frac{1}{4}\left(\frac{a_2}{a_1}\right)^2\right\}=0$$

a_1 and a_2 can be found in terms of a_3 which itself is equal to $\frac{\lambda}{8}$. Thus we obtain the following characteristic equation for ε:

$$\frac{7}{2}\varepsilon^4 - \frac{13}{12}\varepsilon^2 - \frac{15}{16}\lambda + \frac{15}{288} = 0 \qquad .....(10)$$

For $\lambda = 0$ this leads to $\varepsilon = \frac{1}{2}$ in agreement with the value for harmonic oscillators. For large λ, we find

$$\varepsilon \simeq \left(\frac{30}{112}\right)^{\frac{1}{4}} \lambda^{1/4} \simeq 0.7194\, \lambda^{1/4} \qquad .....(11)$$

This may be compared with the exact result

$$\varepsilon \simeq 0.6807\, \lambda^{1/4} + 0.1294\, \lambda^{-1/4} + \cdots$$
$$.....(12)$$

Given λ, the positive roots of the equation (10) will provide the energies of the sextic oscillators. The roots are found by employing the Newton-Raphson method and are listed in table I.

B) The Octic Oscillator : The Schrödinger equation for an octic oscillator is

$$\left\{-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}Kx^2 + \lambda' x^8 - E\right\}\psi(x) = 0$$
$$.....(13)$$

Changing the variable to $y = x\left(\frac{m\omega}{\hbar}\right)^{\frac{1}{2}}$ and putting $\lambda = \frac{\lambda'\hbar^8}{m^4\omega^5}$, $\varepsilon = \frac{E}{\hbar\omega}$, $\omega^2 = \frac{K}{m}$, the equation (13) becomes

$$\left\{\frac{1}{2}\frac{d^2}{dy^2} - \frac{1}{2}y^2 - \lambda y^8 + \varepsilon\right\}\psi(y) = 0$$
$$.....(14)$$

To solve this approximately, we postulate a wave function of the form

$$\psi_0^{(8)}(y) = \text{constant} \times \exp\left[-(b_1 y^4 + b_2 y^6 + b_3 y^8 + b_4 y^{10})^{\frac{1}{2}}\right]$$
$$.....(15)$$

where b_1, b_2, b_3 and b_4 are parameters to be determined.

b_4 is found by solving the equation in the asymptotic region.

For large $|y|$, we obtain

$$\psi_0^{(8)}(y) \sim \exp\left[-\sqrt{\frac{2\lambda}{5}}\, y^5\right] \qquad .....(16)$$

and we conclude $b_4 = \frac{2\lambda}{25}$.

b_1, b_2 and b_3 are determined by solving equation (14) near the origin.

For small $|y|$, we can write

$$\psi_0^{(8)}(y) = \text{constant} \times \exp\left[-(d_2 y^2 + d_4 y^4 + d_6 y^6 + d_8 y^8 + \ldots\ldots)\right]$$
$$.....(17)$$

where $d_2 = b_1^{1/2}$, $d_4 = \frac{1}{2} b_2 b_1^{-1/2}$,

$$d_6 = b_1^{1/2}\left[\frac{1}{2}\frac{b_3}{b_1} - \frac{1}{8}\left(\frac{b_2}{b_1}\right)^2\right],$$

$$d_8 = b_1^{1/2}\left[\frac{1}{2}\frac{b_4}{b_1} - \frac{1}{4}\frac{b_2 b_3}{(b_1)^2} + \frac{1}{16}\left(\frac{b_2}{b_1}\right)^3\right]$$
$$.....(18)$$

Therefore ,

$$\frac{d^2\psi_0^{(8)}}{dy^2} = \{-8d_2(d_2^2 - 3d_4)y^2 + (16d_2 d_4 - 30d_6)y^4 + (24d_2 d_6 + 16d_4^2 - 56d_8)y^6 + \ldots\ldots\}\psi_0^{(8)}$$
$$.....(19)$$

Substituting the expressions for $\psi_0^{(8)}$ and $\frac{d^2\psi_0^{(8)}}{dy^2}$ and setting the coefficients of y^0, y^2, y^4 and y^6 to zero, we get the following equations

$$b_1^{1/2} - \varepsilon = 0$$

$$-6\, b_1^{1/2} b_2 + 4b_1^2 - b_1 = 0$$

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

$$-56\, b_1^{1/2}\left\{\frac{1}{2}\frac{b_4}{b_1} - \frac{1}{4}\frac{b_2 b_3}{b_1^2} + \frac{1}{16}\left(\frac{b_2}{b_1}\right)^3\right\} - b_1\left\{\frac{12 b_3}{b_1} + \left(\frac{b_2}{b_1}\right)^2\right\} = 0$$
$$.....(20)$$

Solving for b_1, b_2, b_3 in terms of $b_4 = \frac{2\lambda}{25}$ and then requiring them to be mutually consistent we derive the following polynomial equation for ε:

$$\frac{632}{135}\varepsilon^5 - \frac{244}{135}\varepsilon^3 + \frac{129}{810}\varepsilon - \frac{28}{25}\lambda = 0$$
$$.....(21)$$

Again, for $\lambda = 0$ we get back $\varepsilon = \frac{1}{2}$ as we should. For large λ we find

$$\varepsilon \simeq 0.7512\, \lambda^{1/5}$$

This compares fairly well with the exact result [4]

$$\varepsilon \simeq 0.70405\, \lambda^{1/5} + \ldots\ldots$$

The energy eigenvalues for different λ calculated by using Newton-Raphson method are listed in table II. The exact values are also listed therein, for comparison.

Discussion

The method of Ginsberg and Montroll apparently works best for small values of λ. This may be understood from the fact that for large λ, the wave function shifts away from the origin and cannot be estimated by the present method. Better agreement with the exact values is seen for sextic than octic oscillator. The asymptotic method proposed by us seems to complement the Ginsberg-Montroll method, as the former yields better agreements for larger values of λ [5]. The present method can be extended to excited states in the straight forward way though computations become involved for third and higher excited states.

Table I
Energy eigenvalues $\mathcal{E}$ of sextic oscillators

λ	Present Method	Exact Values
0.00	0.500000	0.500000
0.001	0.501394	0.501825
0.01	0.512986	0.515443
0.10	0.586616	0.586945
0.50	0.730009	0.717812
1.00	0.825228	0.804966
10.00	1.339464	1.28232
100.00	2.308924	2.19334
1000.00	4.064650	3.85087
20000.00	8.564306	8.10586

Table II
Energy eigenvalues $\mathcal{E}$ of octic oscillators

λ	Present Method	Exact Values
0.00	0.500000	0.500000
0.001	0.504008	0.50543
0.01	0.530199	0.53210
0.10	0.629406	0.62051
1.00	0.852045	0.82069
10.00	1.254959	1.1909
100.00	1.927773	1.8163
1000.00	3.016447	2.8331
20000.00	5.458864	5.1194

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