A New Method for the Energy Eigenstates of Anharmonic Oscillators

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Abstract: ***A new interpolative approximation method is devised for obtaining the eigenvalues and eigenfunctions of anharmonic oscillators. The method is applied to the one-dimensional quartic anharmonic oscillator. The eigenvalues and eigenfunctions are obtained explicitly in the lowest order of approximation. The results are compared with those from other methods. The eigenvalues are found to deviate from the exact values by less than 0.5% for large values of the anharmonic coefficient. Further possible generalisations and higher levels of approximations are also discussed.***

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1. Introduction

The quantum anharmonic oscillators (AHO) have been extensively studied by a variety of methods. It plays an important role as a simple field theory in zero space dimension for which the perturbation series diverges[1,2]. The AHO potential is also employed in nuclear structure, quantum chemistry and quark confinement studies. Among the wide range of methods used for its study mention may be made of WKB method[3], action angle technique [4], Hill determinant method[5], continued fraction method[6], scaled basis method[7], Chebyshev polynomial method[8], variational method[9,10,11], the residue squaring method[12], interpolative perturbation scheme[13], Pade approximants method[14], Uniform asymptotic method[15], Kinetic potentials method[16], the fixed point method[17] and the hepervirial method[18]. The eigenvalues have been obtained to high orders of accuracy by numerical techniques[19,20]. Some others[8,16], have tried to obtain the functional dependence on the anharmonic co-efficient at the cost of numerical accuracy. In the present article, a simple new method that can be easily applied to several types of anharmonic oscillators is presented. The method is applied to the quartic AHO. The method of improving the accuracy is also pointed out. The usefulness of the new method lies not so much in giving better numerical values but in the wide range of applicability and relative simplicity of the techniques involved. The new method is similar in spirit to that of Ginsberg and Montroll[13], but very different in detail.

2. The New Method

We discuss the new method specifically for quartic AHO, though it can be extended to more general AHO's.

The Hamiltonian under consideration is

$$H=\frac{p^2}{2m}+\frac{1}{2}Kx^2+\lambda' x^4 \quad \ldots\ldots\ldots\ldots \quad (1)$$

The Schrodinger equation for the wave function $\psi(x)$ and the eigenvalues E is

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

With the change of variable $y=x\left(\frac{m\omega}{\hbar}\right)^{\frac{1}{2}}$, $\lambda=\frac{\lambda'\hbar}{m^2\omega^2}$, $\omega^2=\frac{K}{m}$ and $\eta=\frac{E}{\hbar\,\omega}$, the Schrodinger equation take the dimensionless form

$$\left(\frac{1}{2}\frac{d^2}{dy^2}+\eta-\frac{1}{2}y^2-\lambda y^4\right)\psi(y)=0 \quad \ldots\ldots\ldots (3)$$

To start with, we consider the ground state of AHO. The wave function $\psi_0(y)$ for small $|y|$ is easily found to be

$$\psi_0(y)>e^{[-(\eta y^2)+O(y^4)]} \quad \ldots\ldots\ldots (4)$$

For large $|y|$ the asymptotic solution to equation (3) is

$$\psi_0(y)>e^{[-\beta|y|^3+O|y|]} \quad \ldots\ldots\ldots\ldots\ldots\ldots (5)$$

Where $\beta^2=\frac{2\lambda}{9}$.

Hence we postulate the following interpolative function that has the correct behaviour for small and large $|y|$ to represent the ground state:

$$\psi_0(y)=e^{\left[-(\eta y^8+b(\lambda)y^{10}+c(\lambda)y^{12})^{\frac{1}{4}}\right]} \quad \ldots\ldots\ldots (6)$$

Where $b(\lambda)$ and $c(\lambda)$ are some functions of λ to be determined.

Now we demand that $\psi_0(y)$ of equation (6) satisfy the equation (3) in the large $|y|$ region.

For large $|y|$, we can put

$$\psi_0(y)>e^{\left[-c^{1/4}\left\{|y|^3+\frac{b}{4c}|y|+\left(\frac{\eta^4}{4c}-\frac{3\,b^2}{32\,c^2}\right)|y|^{-1}+O|y|^{-3}\right\}\right]} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (7)$$

Therefore

$$\frac{d\psi_0}{dy}>-c^{1/4}\left[3y^2+\frac{b}{4c}-\left(\frac{\eta^4}{4c}-\frac{3}{32}\frac{b^2}{c^2}\right)y^{-2}+O(y^{-4})\right]\psi_0(y) \ldots (8)$$

and

$$\frac{d^2\psi_0}{dy^2}>$$

$$c^{1/2}\left[3y^2+\frac{b}{4c}-\left(\frac{\eta^4}{4c}-\frac{3}{32}\frac{b^2}{c^2}\right)y^{-2}+O(y^{-4})\right]^2\psi_0(y)$$
$$-c^{1/4}\left[6y+2\left(\frac{\eta^4}{4c}-\frac{3}{32}\frac{b^2}{c^2}\right)y^{-3}+O(y^{-5})\right]\psi_0(y)$$
$$\ldots\ldots\ldots..(9)$$

Substituting equation (9) into equation (3) and equating the coefficients of y^2, y^4 and y^0 to zero we find the following equations:

$$\frac{9}{2}c^{1/2}-\lambda=0\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(10)$$
$$\left(\frac{3}{4}b\,c^{-1/2}-\frac{1}{2}\right)=0\ldots\ldots\ldots\ldots\ldots\ldots..(11)$$
$$3c^{1/2}\left(\frac{1}{4}\eta^4c^{-1}-\frac{3}{32}b^2c^{-2}\right)-\frac{1}{32}b^2c^{-\frac{3}{2}}$$
$$=\eta\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots.(12)$$

The terms that are dropped are $O(y^{-2})$ and smaller and are negligible for $|y|^2 \gg \lambda^{-\frac{1}{2}}$. Hence the method works best for large λ.

Solving equations (10), (11) and (12) we find

$$c={4\lambda^2}/{81},\ b={4\lambda}/{27}$$

and the characteristic equation for η :

$$27\eta^4-8\lambda\eta-5=0\ldots\ldots\ldots\ldots\ldots\ldots.(13)$$

This equation may be compared with that of Ginsberg and Montroll [13] who derive it by matching the coefficients near the origin. In the lowest order, they get

$$\eta^3-\frac{1}{4}\eta-\frac{\lambda}{3}=0.$$

The positive roots of equation (13) will provide the energy values for a given λ. It is now quite straightforward to generalize the new method to other AHO's.

3. Results and Discussion

Equation (3) can be solved[20] in a decreasing power series for large λ as:

$$\eta=a_1\lambda^{\frac{1}{3}}+a_2\lambda^{-\frac{1}{3}}+a_3\lambda^{-1}+\ \ldots\ldots\ldots$$

Substituting such a series in (13) and comparing coefficients of $\lambda^{4/3},\lambda^{2/3},\lambda^0$ etc, we find that

$$\eta > 0.66667\lambda^{1/3}+0.20833\lambda^{-1}+\ \ldots\ldots$$

which can be compared with exact result (Hioe, 1975):

$$\eta > 0.667986\lambda^{1/3}+0.14367\lambda^{-1/3}+\ \ldots\ldots$$

Hence the lowest order approximation of our method leads to energies that deviate by less than 0.4% from exact values for $\lambda \geq 1000$. The positive roots of the equation (13) have been calculated using Newton-Raphson method for several values of λ. The results are listed and compared with those from other methods in table-1. It can be seen that our method gives energies in far better agreement with the exact values than that of the Ginsberg and Montroll in the first approximation[13] for all values of $\lambda \geq 1.0$. By postulating $\psi_0(y)$ that includes three, four and more number of functions of λ instead of just two, in the following forms:

$$\psi_0^{(2)}(y) > e^{\left[-\left(\eta^6y^{12}+a(\lambda)y^{14}+b(\lambda)y^{16}+c(\lambda)y^{18}\right)^{1/6}\right]}$$

and

$$\psi_0^{(3)}(y) > e^{\left[-\left(\eta^8y^{16}+a(\lambda)y^{18}+b(\lambda)y^{20}+c(\lambda)y^{22}+d(\lambda)y^{24}\right)^{1/8}\right]}$$

it is clearly possible to improve the accuracy for smaller λ .

By considering the products of $\psi_0(y)$ with various polynomials of y the excited states can be worked out. These and other applications of the method are under study and will be reported in due course.

Table 1: Ground state energies of a quartic AHO:

η / λ	Our method	Ginsberg and Montroll[13] in first approximation	Exact values [20]
0.05	0.66455	0.531	0.53264
0.1	0.67298	0.557	0.55915
0.5	0.73654	0.699	0.69618
1.0	0.80709	0.813	0.80337
2.0	0.92548	0.969	0.95157
50.0	2.46017	2.568	2.4997
200.0	3.89973	4.075	3.9209
1000.0	6.66687	6.946	6.6942
8000.0	13.3334	13.873	13.3669
20000.0	18.0961	18.825	18.1372

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