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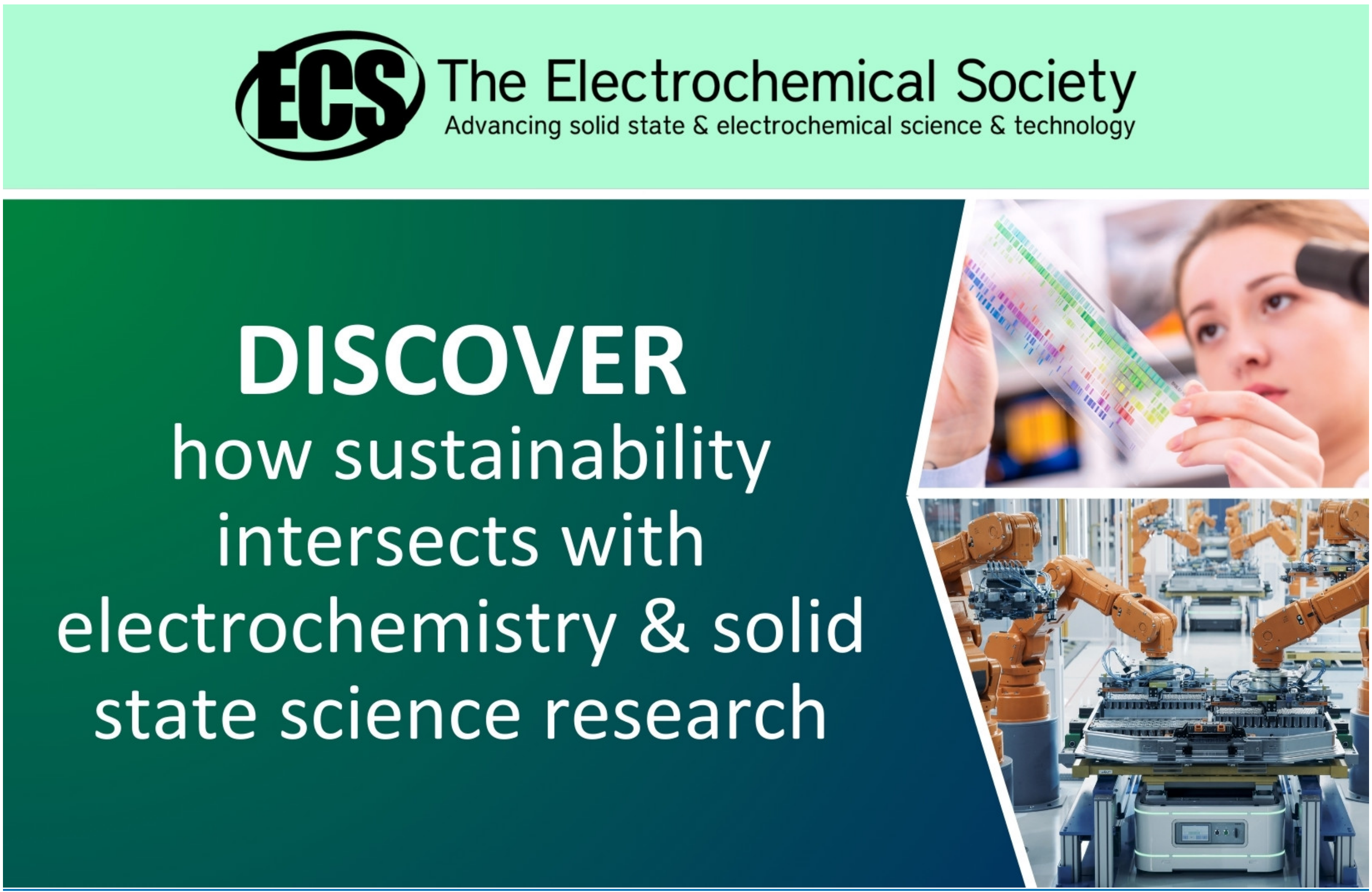

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Analytic ground state energy and wave function of a quantum system in an exponential-form anharmonic interaction potential

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Abstract. An anharmonic oscillator with a perturbed quadratic potential which is coupled with an exponential term is being investigated in this paper by isolating an anharmonic oscillator interaction potential from the actual interaction experienced by the quantum system studied, and using standard perturbative techniques. The anharmonic potential considered is of interest because of its usefulness in the study of non-centrosymmetric materials which have applications in piezoelectricity. The ground state energy eigenvalue and its associated eigenstates were calculated for the quantum system using an analytical approach. Results obtained are compared to those of quantised harmonic oscillator to show the effect of the perturbation.

Keywords: anharmonic oscillator, perturbation theory, non-centrosymmetric materials

1. Introduction

The Schrödinger equation is solvable for a limited number of systems and among them is the quantum harmonic oscillator, however, in nature, where only real systems exist, this equation does not have a solution except for that of the hydrogen atom. [1, 2, 3]. In previous studies, anharmonic oscillators with cubic, sextic and decatic potentials have been solved using different numerical methods [3, 4, 5, 6, 7]. The perturbation theory is one of the methods to find solutions to the Schrödinger equation of an anharmonic oscillator [1, 9]. An alternative approach to this method was developed in [8] and was used to solve a system with quadratic perturbations. This method was compared to the Rayleigh-Schrödinger theory and was reported to contain results of the time independent case and the time dependent parameters served to time evolutions of the correctness [8].Other methods like the Dirac operator technique and Fourth order Runge-Kutta method within the Numerov approach were also used to study quartic anharmonic oscillators due to their simplicity and robust nature. Furthermore, it was stated that the asymptotic iteration method is a more efficient but rigorous approach for obtaining wave functions of anharmonic systems especially those without exact solutions [4].

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In this study, an analytical approach has been used to find ground state wave function and eigenvalue of an anharmonic oscillatorwith quadratic-exponential form perturbation term and bounded at infinity.This was achieved by employing the first order perturbation theory and also standard integral definitions [10]. This kind of anharmonic potential can be used to study non-centrosymmetric materials which have applications in piezoelectricity [11, 12].

2. Perturbation Theory

The one-dimensional time-independent Schrödinger equation is a basic and essential step towards the calculation of the eigenvalues (energies) of an anharmonic oscillator [3]. Thus, in general, the one-dimensional time-independent Schrödinger equation is given as:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_n(x)}{dx^2} + V(x)\psi_n(x) = E_n\psi_n(x) \quad (1)$$

where $\psi_n(x)$ is wave function,$V(x)$ is the potential energy and E_n is the corresponding energy eigenvalue.

For an ideal system, equation (1) can be rewritten as

$$H^0\psi_n^0 = E_n^0\psi_n^0 \quad (2)$$

Now suppose that equation (2) is solved, a complete set of orthonormal eigenfunctions, ψ_n^0(where the superscript 0 represents an unperturbed quantity) are obtained, that is,

$$\langle\psi_n^0|\psi_m^0\rangle = \delta_{nm} \quad (3)$$

with their corresponding energy eigenvalues, $E_n^0$and $\delta_{nm}$is the kronecker delta. However, when the system is slightly perturbed, there is a new equation,

$$H\psi_n = E_n\psi_n \quad (4)$$

such that

$$H = H^0 + \epsilon H^{'} \quad (5)$$

where $H^{'}$ is the perturbation and $0 < \epsilon < 1$. The first-order correction to the nth eigenvalue, E_n^1 also known as the expectation value of the perturbation is given as

$$E_n^1 = \langle\psi_n^0|H^{'}|\psi_n^0\rangle \quad (6)$$

Likewise, the first-order correction to the wave function is given as

$$\psi_n^1 = \sum_{m\neq n}^{N}\frac{\langle\psi_m^0|H^{'}|\psi_n^0\rangle}{(E_n^0 - E_m^0)}|\psi_m^0\rangle \quad (7)$$

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Thus, the perturbed wave function corrected to the first order is given as

$$\boldsymbol{\psi_n = \psi_n^0 + \psi_n^1} \tag{8}$$

while the corresponding perturbed eigenvalue value corrected to the first order is given as

$$\boldsymbol{E_n = E_n^0 + \langle \psi_n^0 | H^{'} | \psi_n^0 \rangle} \tag{9}$$

3. Problem Formulation

Consider an ideal harmonic oscillator,

$$\boldsymbol{V(x) = \frac{1}{2} kx^2} \tag{10}$$

but for the purpose of this paper, we introduce a perturbation to give rise to the anharmonic potential,

$$\boldsymbol{V(x) = \frac{1}{2} kx^2 + \frac{1}{16}(x + x^2)e^{rx}} \tag{11}$$

and $\boldsymbol{k = m\omega^2}$, k > 0 and r > 0 are constants, m is the mass of the particle and ω is the angular frequency. Figure (1) shows the plot for both the harmonic and anharmonic potentials. From the graph, it can be seen that close to the equilibrium point the plots coincide despite the presence of perturbation, however, at larger distances, the effect of perturbation is more pronounced. From equation (11), the perturbation term is

$$\boldsymbol{H^{'} = \frac{1}{16}(x + x^2)e^{rx}} \tag{12}$$

and it can be seen that it consists of both a quadratic term coupled with an exponential factor.

The anharmonic potential (12) does not satisfy the equation, V(x) = V(-x) which makes it promising for the study of non-centrosymmetric materials [11]. Non-centrosymmetric materials do not have points of inversion symmetry throughout their volume and are important in the study of piezoelectric materials [12].

Also, the non-zero ground state energy of the harmonic oscillator is

$$\boldsymbol{E_0 = \frac{1}{2}\hbar\omega} \tag{13}$$

while the ground state wave function of the harmonic oscillator is given as

$$\boldsymbol{\psi_0^0(x) = \left(\frac{\alpha}{\pi}\right)^{\frac{1}{4}} e^{-\frac{\alpha x^2}{2}}} \tag{14}$$

where $\boldsymbol{\alpha = 2m\pi\nu/\hbar}$, $\hbar$ is the Planck's constant, m is the mass and$\boldsymbol{\nu}$ is the frequency.

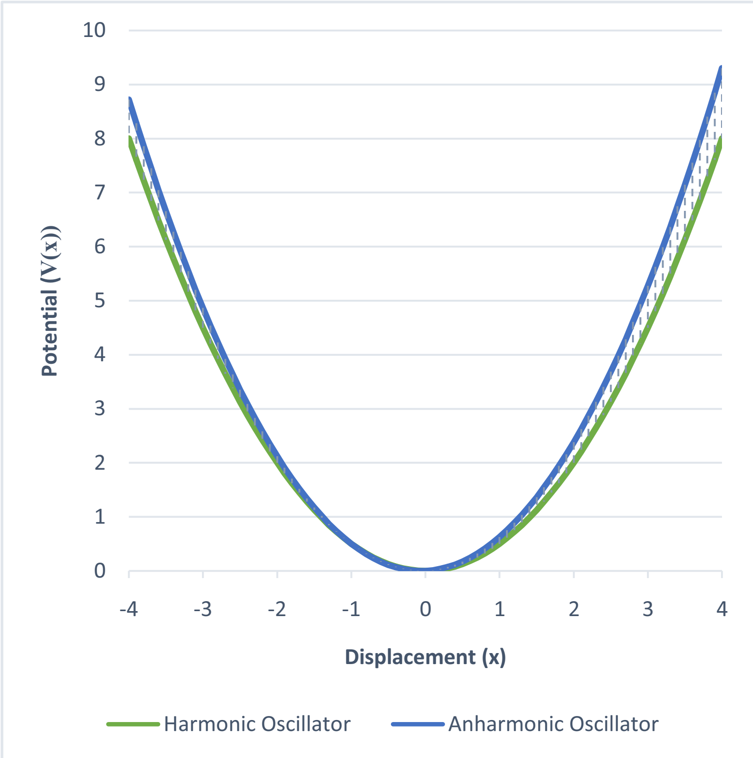

Figure 1: Graph of potential against displacement for the harmonic and the anharmonic oscillator

4.Calculations and Results

(a) Perturbed Eigenvalue Calculation

Substituting equation (6) into equations (13) and (14) and writing in integral form, hence, the following calculations:

$$\boldsymbol{E_n^1 = \int_{-\infty}^{\infty} \psi_n^{(0)} H' \psi_m^{(0)^*} dx} \tag{15}$$

$$\boldsymbol{E_n^1 = \int_{-\infty}^{\infty} \left(\frac{\alpha}{\pi}\right)^{\frac{1}{4}} e^{-\frac{\alpha x^2}{2}} H' \left(\frac{\alpha}{\pi}\right)^{\frac{1}{4}} e^{-\frac{\alpha x^2}{2}} dx} \tag{16}$$

$$\boldsymbol{E_n^1 = \left(\frac{\alpha}{\pi}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} e^{-\frac{\alpha x^2}{2}} \left(\frac{1}{16}(x + x^2) e^{rx}\right) e^{-\frac{\alpha x^2}{2}} dx} \tag{17}$$

$$E_n^1 = \frac{1}{16}\left(\frac{\alpha}{\pi}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} e^{-\alpha x^2}(x + x^2)e^{rx}dx \tag{18}$$

$$E_n^1 = \frac{1}{16}\left(\frac{\alpha}{\pi}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} xe^{-\alpha x^2+2\left(\frac{r}{2}\right)x} + x^2 e^{-\alpha x^2+2\left(\frac{r}{2}\right)x}dx \tag{19}$$

Using the standard integrals [10],

$$\int_{-\infty}^{\infty} xe^{-px^2+2qx}\,dx = \frac{q}{p}\sqrt{\frac{\pi}{p}}e^{\frac{q^2}{p}} \tag{20}$$

And

$$\int_{-\infty}^{\infty} x^2 e^{-\mu x^2+2\nu x}\,dx = \frac{1}{2\mu}\sqrt{\frac{\pi}{\mu}}\left(1 + \frac{2v^2}{\mu}\right)e^{\frac{v^2}{\mu}} \tag{21}$$

Thus, equation (19) becomes

$$E_n^1 = \frac{1}{16}\left[\frac{r/2}{\alpha}e^{\frac{r^2/4}{\alpha}} + \frac{1}{2\alpha}\left(1 + \frac{r^2/2}{\alpha}\right)e^{\frac{r^2/4}{\alpha}}\right] \tag{22}$$

Since $\alpha = 2m\pi v/\hbar$, then equation (22) becomes

$$E_n^1 = \frac{r\hbar}{64m\pi v}e^{\frac{\hbar r^2}{8m\pi v}} + \frac{\hbar}{64m\pi v}\left(\frac{4m\pi v + \hbar r^2}{4m\pi v}\right)e^{\frac{\hbar r^2}{8m\pi v}} \tag{23}$$

$$E_n^1 = \frac{\hbar}{64m\pi v}\left[1 + r + \frac{\hbar r^2}{4m\pi v}\right]e^{\frac{\hbar r^2}{8m\pi v}} \tag{24}$$

Hence, using the fact that the eigenvalue of an ideal harmonic oscillator is given as$1/2\hbar\omega$, thus,

$$E_n = \frac{1}{2}\hbar\omega + \frac{\hbar}{64m\pi v}\left[1 + r + \frac{\hbar r^2}{4m\pi v}\right]e^{\frac{\hbar r^2}{8m\pi v}} \tag{25}$$

Using the first order perturbation theory for the correction of the energy we have equation (25).

(b) Perturbed Wave Function Calculation

The first four wave functions of the simple harmonic oscillators [1] are given by

$$\psi_0 = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2} \tag{26}$$

$$\psi_1 = \left(\frac{\alpha}{\pi}\right)^{1/4} \sqrt{2\alpha}xe^{-\alpha x^2/2} \tag{27}$$

$$\psi_2 = \left(\frac{\alpha}{\pi}\right)^{1/4} \frac{1}{\sqrt{2}}(2\alpha x^2 - 1)e^{-\alpha x^2/2} \tag{28}$$

$$\psi_3 = \left(\frac{\alpha}{\pi}\right)^{1/4} \frac{1}{\sqrt{3}}(2\alpha^{3/2}x^3 - 3\alpha^{1/2}x)e^{-\alpha x^2/2} \tag{29}$$

and the energy eigenvalues are

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \quad , \; n = 0, 1, 2, 3, \dots \tag{30}$$

In this section, another standard integral [10]was employed:

$$\int_{-\infty}^{\infty} x^n e^{-px^2+2qx}\, dx = n!\, e^{-q^2/p}\sqrt{\frac{\pi}{\alpha}}\left(\frac{q}{p}\right)^n \sum_{k=0}^{[n/2]} \frac{1}{(n-2k)!k!}\left(\frac{p}{4q^2}\right)^k \tag{31}$$

To calculate the first order correction to the wave function, equation (7), the following terms are first computed which will then be substituted back into equation (7):

$$\frac{\langle\psi_0^0|H'|\psi_1^0\rangle}{E_1 - E_0} = \frac{1}{\hbar\omega}\int_{-\infty}^{\infty}\left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2}\left(\frac{1}{16}(x + x^2)e^{rx}\right)\left(\frac{\alpha}{\pi}\right)^{1/4}\sqrt{2\alpha}\, x e^{-\alpha x^2/2} dx \tag{32}$$

$$= \frac{1}{16\hbar\omega}(2\alpha)^{1/2}\left(\frac{\alpha}{\pi}\right)^{1/2}\int_{-\infty}^{\infty}(x^2 + x^3)\, e^{-\alpha x^2} e^{rx} dx \tag{33}$$

$$= \frac{1}{16\hbar\omega}(2\alpha)^{1/2}\left(\frac{\alpha}{\pi}\right)^{1/2}\int_{-\infty}^{\infty}\left(x^2 e^{-\alpha x^2+2(r/2)} + x^3 e^{-\alpha x^2+2(r/2)}\right) dx \tag{34}$$

$$= \frac{1}{16\hbar\omega}(2\alpha)^{1/2}\left(\frac{\alpha}{\pi}\right)^{1/2}\left[\frac{1}{2}\sqrt{\frac{\pi}{\alpha}}\left(1 + \frac{r^2}{2\alpha}\right)e^{-r^2/4\alpha} + 3!\, e^{-r^2/4\alpha}\sqrt{\frac{\pi}{\alpha}}\left(\frac{r^3}{8\alpha}\right)\sum_{k=0}^{1}\frac{1}{(3-2k)!k!}\left(\frac{\alpha}{r^2}\right)^k\right] \tag{35}$$

$$= \frac{1}{16\hbar\omega}(2\alpha)^{1/2}\left(\frac{\alpha}{\pi}\right)^{1/2}\left[\frac{1}{2}\sqrt{\frac{\pi}{\alpha}}\left(1 + \frac{r^2}{2\alpha}\right)e^{-r^2/4\alpha} + 6e^{-r^2/4\alpha}\sqrt{\frac{\pi}{\alpha}}\left(\frac{r^3}{8\alpha}\right)\left(\frac{1}{3} + \frac{\alpha}{r^2}\right)\right] \tag{36}$$

$$\frac{\langle\psi_0^0|H'|\psi_2^0\rangle}{E_2 - E_0} = \frac{1}{2\hbar\omega}\int_{-\infty}^{\infty}\left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2}\left(\frac{1}{16}(x + x^2)e^{rx}\right)\left(\frac{\alpha}{\pi}\right)^{1/4}\frac{1}{\sqrt{2}}(2\alpha x^2 - 1)e^{-\alpha x^2/2} dx \tag{37}$$

$$= \frac{1}{32\hbar\omega}\left(\frac{\alpha}{\pi}\right)^{1/2}\int_{-\infty}^{\infty}(2\alpha x^3 - x + 2\alpha x^4 + x^2)\, e^{-\alpha x^2+2(r/2)} dx \tag{38}$$

$$= \frac{1}{32\hbar\omega}\left(\frac{\alpha}{\pi}\right)^{1/2}\left[12\alpha e^{-r^2/4\alpha}\sqrt{\frac{\pi}{\alpha}}\left(\frac{r^3}{8\alpha}\right)\left[\frac{1}{3} + \frac{\alpha}{r^2}\right] - \left(\frac{r}{2\alpha}\right)\sqrt{\frac{\pi}{\alpha}}\, e^{-\frac{r^2}{4\alpha}} + \right.$$

2α4!e−r2/4απαr38αk=0214−2k!k!αr2k−12απα1+r24 (39)

$$= \frac{1}{32\hbar\omega}\left(\frac{\alpha}{\pi}\right)^{1/2}\left[12\alpha e^{-r^2/4\alpha}\sqrt{\frac{\pi}{\alpha}}\left(\frac{r^3}{8\alpha}\right)\left[\frac{1}{3}+\frac{\alpha}{r^2}\right]-\left(\frac{r}{2\alpha}\right)\sqrt{\frac{\pi}{\alpha}}e^{-\frac{r^2}{4\alpha}}-\frac{1}{2\alpha}\sqrt{\frac{\pi}{\alpha}}\left(1+\frac{r^2}{4}\right)+\right.$$

48αe−r2/4αr416α4πα124+12αr2+12αr22 (40)

$$\frac{\langle\psi_0^0|H'|\psi_3^0\rangle}{E_3-E_0} = \frac{1}{3\hbar\omega}\int_{-\infty}^{\infty}\left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2}\left(\frac{1}{16}(x+x^2)e^{rx}\right)\left(\frac{\alpha}{\pi}\right)^{1/4}\frac{1}{\sqrt{3}}\left(2\alpha^{\frac{3}{2}}x^3-3\alpha^{\frac{1}{2}}x\right)e^{-\alpha x^2/2}dx \tag{41}$$

$$= \frac{1}{48\hbar\omega}\frac{1}{\sqrt{3}}\left(\frac{\alpha}{\pi}\right)^{1/2}\int_{-\infty}^{\infty}\left(2\alpha^{\frac{3}{2}}x^4-3\alpha^{\frac{1}{2}}x^2+2\alpha^{\frac{3}{2}}x^5-3\alpha^{\frac{1}{2}}x^3\right)e^{-\alpha x^2+2(r/2)} \tag{42}$$

$$= \frac{1}{48\hbar\omega}\frac{1}{\sqrt{3}}\left(\frac{\alpha}{\pi}\right)^{1/2}\left[2\alpha^{\frac{3}{2}}\left[48\alpha e^{-r^2/4\alpha}\left(\frac{r^4}{16\alpha^4}\right)\sqrt{\frac{\pi}{\alpha}}\left(\frac{1}{24}+\frac{1}{2}\left(\frac{\alpha}{r^2}\right)+\frac{1}{2}\left(\frac{\alpha}{r^2}\right)^2\right)\right]-3\alpha^{\frac{1}{2}}\left[\frac{1}{2\alpha}\sqrt{\frac{\pi}{\alpha}}\left(1+\right.\right.\right.$$

r24e−r24α−
3α126e−r24απαr38α13+αr2+2α324!e−r2/4απαr532α5k=0215−2k!k!αr2k (43)

$$= \frac{1}{48\hbar\omega}\frac{1}{\sqrt{3}}\left(\frac{\alpha}{\pi}\right)^{1/2}\left[2\alpha^{\frac{3}{2}}\left[48\alpha e^{-r^2/4\alpha}\left(\frac{r^4}{16\alpha^4}\right)\sqrt{\frac{\pi}{\alpha}}\left(\frac{1}{24}+\frac{1}{2}\left(\frac{\alpha}{r^2}\right)+\frac{1}{2}\left(\frac{\alpha}{r^2}\right)^2\right)\right]-3\alpha^{\frac{1}{2}}\left[\frac{1}{2\alpha}\sqrt{\frac{\pi}{\alpha}}\left(1+\right.\right.\right.$$

r24e−r24α−3α126e−r24απαr38α13+αr2+240α32e−r24απαr532α51120+16αr2+12αr22 (44)

Hence, substituting equations [36], [40] and [44] into equation (7)and then computing to get

$$\psi_0^1 = \frac{1}{16\hbar\omega}\left[\left[\sqrt{2\alpha}\left(\frac{1}{2\alpha}\left(1+\frac{r^2}{4}\right)+6\left(\frac{r^3}{8\alpha}\right)\left(\frac{1}{3}+\frac{\alpha}{r^2}\right)\left(1+\frac{\alpha}{\sqrt{2}}\right)\right)-\frac{r}{4\sqrt{2\alpha}}+24\alpha\left(\frac{r^4}{16\alpha^4}\right)\left(\frac{1}{24}+\right.\right.\right.$$

12αr2+12αr2212+433α32−1+r24142α+α1223α−α1235r54α51120+16αr2+12αr22+…e−r24ααπ1/4e−αx2/2 (45)

Thus, the ground state wave function of the anharmonic oscillator using the first-order correction is given by equation (46)

$$\psi_0 = \left(\frac{\alpha}{\pi}\right)^{1/4}e^{-\alpha x^2/2}+\frac{1}{16\hbar\omega}\left(\frac{\alpha}{\pi}\right)^{1/4}e^{-\alpha x^2/2}\left[\left[\sqrt{2\alpha}\left[\frac{1}{2\alpha}\left(1+\frac{r^2}{4}\right)+6\left(\frac{r^3}{8\alpha}\right)\left(\frac{1}{3}+\frac{\alpha}{r^2}\right)(1+\alpha)\right]-\frac{r}{4\alpha}-\left(\frac{1}{3}+\frac{\alpha}{r^2}\right)\left(\frac{1}{4\alpha}+\frac{\alpha^{\frac{1}{2}}}{2\alpha}\right)-\alpha^{\frac{1}{2}}\left[\left(\frac{5r^5}{4\alpha^5}\right)\left(\frac{1}{120}+\frac{1}{6}\left(\frac{\alpha}{r^2}\right)+\frac{1}{2}\left(\frac{\alpha}{r^2}\right)^2\right)\right]+\cdots\right]e^{-\frac{r^2}{4\alpha}}\right] \tag{46}$$

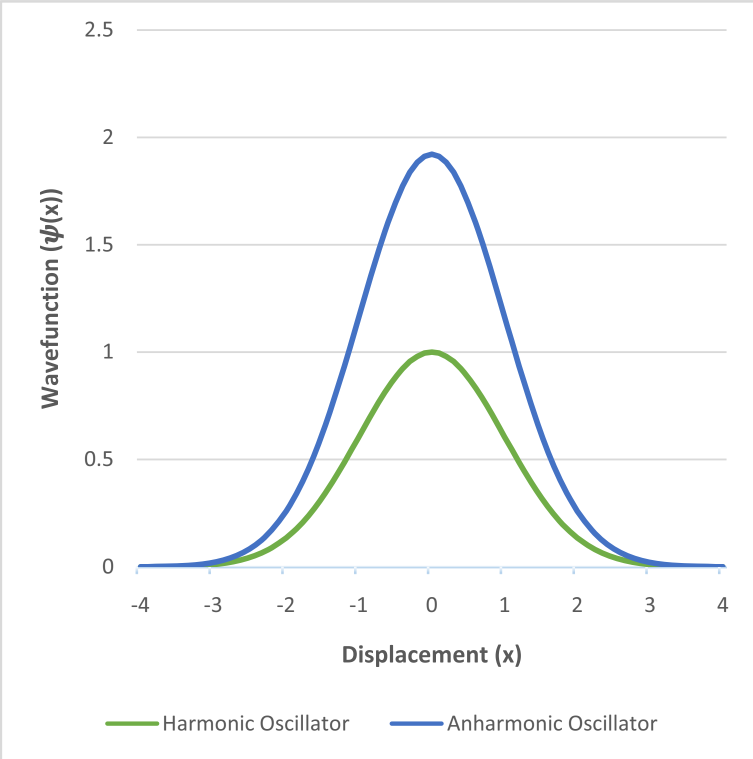

Figure 2: Graph of wave function against displacement for the harmonic and the anharmonic oscillator

For this calculation, we have only used the first four terms of the simple harmonic oscillator, hence the reason for the ellipsis. Since $\boldsymbol{\alpha}$ and r are basically constants, we can rewrite equation (46) as

$$\boldsymbol{\psi_0} = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2} + \frac{A}{16\hbar\omega} e^{-\frac{r^2}{4\alpha}} \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2} \tag{47}$$

$$\boldsymbol{\psi_0} = \left(\frac{\alpha}{\pi}\right)^{1/4} \left(1 + \frac{A}{16\hbar\omega} e^{-\frac{r^2}{4\alpha}}\right) e^{-\alpha x^2/2} \tag{48}$$

This means that in comparison with the unperturbed wave function, the perturbed wave function differs by a factor of $(\mathbf{1} + \boldsymbol{A}/\boldsymbol{\hbar\omega})$which represents the terms in the largest parentheses in equation (46). The plot of equations (26) and (48) is shown in figure (2), for simplicity, the values of the arbitrary constants have been set to one. In general, the perturbed wave function has a similar trend to the unperturbed wave function although the former has a higher amplitude.

5. Conclusion

In quantum mechanics, it is imperative to find solutions to the Schrödinger equation of the system considered. However, in nature most systems differ from the ideal, a method like the perturbation theory comes in handy in finding solutions to the perturbed systems. In this study, the first order energy correction and the ground state wave function of an anharmonic oscillator has been obtained analytically using definite integrals. The integral definition makes it easy to solve the problems and hence is a powerful tool for this kind of problems, provided the integral definition already exist in literature. This calculation can be extended to calculate the second order energy correction and also other excited states wave functions which is still an ongoing research.

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