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Quantum Mechanical Anharmonic Oscillator

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Abstract

In this article the Schrödinger wave equation of quantum mechanical anharmonic oscillator with potential energy $V(x) = Ax^4$ has been analytically solved. It is shown that the corresponding wave functions perturb from that of simple quantum harmonic oscillator, i.e. they are basically Hermite polynomials plus a power series of x. The corresponding energy levels have maximum width at the bottom of the well while become narrower as they come up and squeeze at the top of it, in contrast to the energy levels of simple quantum harmonic oscillator.

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Introduction

Yet, the Schrödinger equation is used to describe many quantum mechanical systems, although it cannot be solved except for some simple models. This equation is simply a second order variable coefficient linear differential equation that can be solved exactly by ”brute force” using the method of power series expansion from differential equations or by using ladder operators from quantum mechanics. However, the anharmonic oscillator cannot be solved exactly and some of the ideas of quantum mechanical perturbation theory must be used [1,2].

The Schrödinger wave equation for the anharmonic oscillator discussed in this paper is:

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(z) + Az^4\Psi(z) = E\Psi(z)$$

To solve this equation in one dimension we first use a second order linear differential equation. Then a power series solution is used to solve it. Inserting the power series in the differential equation and because they are independent summations we demand that the remaining net coefficients vanish.

Once this is done the *recurrence relation* is obtained and becomes possible to compute the coefficients in the expansion of the series solution.

This paper is organized as follows. In Section 1 a second order differential equation leading to a differential equation for a quantum mechanical anharmonic oscillator is given. In Section 2 we develop analytical solutions based on power series method. The coefficients in the resulting series are then used to introduce the wave functions and energy levels in Section 3.

Motivation

We introduce the second-order linear differential equation

$$y'' - 2xy' + (2n + x^2 - x^4)y = 0 \tag{1}$$

which is clearly not self adjoint. It is convenient to introduce a set of unnormalised functions φ_n by

$$\varphi_n = e^{-x^2/2} y(x) \tag{2}$$

Substituting into Eq. (1) yields the differential equation for φ_n

$$\varphi_n'' + (2n + 1 - x^4)\varphi_n = 0 \tag{3}$$

This is the differential equation for a quantum mechanical anharmonic oscillator with an energy potential $V(x) = Ax^4$.

Analytical solution

By using the method of series solution we wish to solve Eq. (1). Trying

$$y(x) = x^k\left(a_0 + a_1 x + a_2 x^2 + a_3 x^3 + \cdots\right) = \sum_{m=0}^{\infty} a_m x^{k+m}, \quad a_0 \neq 0, \tag{4}$$

which the exponent k and all the coefficients a_m to be determined. By differentiating twice it gives

$$\frac{dy}{dx} = \sum_{m=0}^{\infty} a_m (k+m) x^{k+m-1},$$

$$\frac{d^2 y}{dx^2} = \sum_{m=0}^{\infty} a_m (k+m)(k+m-1) x^{k+m-2},$$

By substituting into Eq. (1) one has

$$\sum_{m=0}^{\infty} a_m (k+m)(k+m-1) x^{k+m-2} - 2\sum_{m=0}^{\infty} a_m (k+m) x^{k+m} + 2n\sum_{m=0}^{\infty} a_m x^{k+m} + \sum_{m=0}^{\infty} a_m x^{m+k+2} - \sum_{m=0}^{\infty} a_m x^{m+k+4} = 0 \tag{5}$$

The lowest power of x appearing in Eq. (5) is x^{k-2}, for $m = 0$ in the first summation. The uniqueness of power series requires that the coefficient vanish which yields

$$a_0 k(k-1) = 0$$

By definition, $a_0 \neq 0$, therefore one obtains

$$k(k-1)=0 \tag{6}$$

This is the so called indicial equation that requires either $k=0$ or $k=1$.

For the present we return to Eq. (5) and set $m=j+2$ in the first summation, $m=j$, $m=j$, $m=j-2$ and $m=j-4$ in the second, third, forth and fifth summations respectively. This gives

$$a_{j+2}(k+j+2)(k+j+1)-2a_j(k+j-n)+a_{j-2}-a_{j-4}=0$$

$$a_{j+2}=\frac{a_{j-4}-a_{j-2}+2a_j(k+j-n)}{(k+j+2)(k+j+1)} \tag{7}$$

By repeating application of this recurrence relation one obtains

For $k=0$

$$a_2=\frac{a_0}{2!}2(-n) \qquad \text{(even j)}$$

$$a_4=\frac{a_0}{4!}\left[-2!+2^2(-n)(2-n)\right]$$

$$a_6=\frac{a_0}{6!}\left[4!-\frac{4!}{2!}2(-n)-2^2(4-n)+2^3(-n)(2-n)(4-n)\right]$$

And for $k=1$

$$a_2=\frac{a_0}{3!}2(1-n) \qquad \text{(even j)}$$

$$a_4=\frac{a_0}{5!}\left[-3!+2^2(1-n)(3-n)\right]$$

Putting these coefficients (for case $k=0$) into Eq. (4), one has

$$y_{even}=a_0\Bigg[1+\frac{1}{2!}(2(-n))x^2+\frac{1}{4!}\left(-2!+2^2(-n)(2-n)\right)x^4 + \frac{1}{6!}\left(4!-\frac{4!}{2!}2(-n)-2^2(4-n)+2^3(-n)(2-n)(4-n)\right)x^6+\cdots\Bigg]$$

Now separating the Hermite polynomials (for even n) and pulling out various parameters:

$$y_{even}=a_0\left[1+\frac{1}{2!}(2(-n))x^2+\frac{1}{4!}\left(2^2(-n)(2-n)\right)x^4+\frac{1}{6!}\left(2^3(-n)(2-n)(4-n)\right)x^6+\cdots\right] + a_0\left[-\frac{2!}{4!}x^4+\frac{1}{6!}\left(4!-\frac{4!}{2!}2(-n)-2^2(4-n)\right)x^6+\cdots\right] \tag{8}$$

And doing the same (for odd Hermite polynomials) for $k=1$

$$y_{odd}=a_0\left[x+\frac{1}{3!}(2(1-n))x^3+\frac{1}{5!}\left(2^2(1-n)(3-n)\right)x^5+\frac{1}{7!}\left(2^3(1-n)(3-n)(5-n)\right)x^7+\cdots\right] + a_0\left[-\frac{3!}{5!}x^5+\frac{1}{7!}\left(5!-\frac{5!}{3!}2(1-n)-3!\times 2(5-n)\right)x^7+\cdots\right]$$

Noting that the first brakets of the right hand sides y_{even} and y_{odd} are just Hermite polynomial and inserting it in Eq. (2), for even n one obtains

$$\varphi_n(x) = e^{-x^2/2}\left\{H_n(x) + a_0 x^4\left[-\frac{2!}{4!} + \frac{1}{6!}\left(4! - \frac{4!}{2!}2(-n) - 2^2(4-n)\right)x^2 + \cdots\right]\right\} \tag{9}$$

And for odd n

$$\varphi_n(x) = e^{-x^2/2}\left\{H_n(x) + a_0 x^5\left[-\frac{3!}{5!} + \frac{1}{7!}\left(5! - \frac{5!}{3!}2(1-n) - 3!\times 2(5-n)\right)x^2 + \cdots\right]\right\}$$

The wave functions and energy levels

For a potential energy $V(x) = Ax^4$ the Schrödinger wave equation is

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(z) + Az^4\Psi(z) = E\Psi(z) \tag{10}$$

Assuming a particle with mass m a total energy E, and using the abbreviations

$$x = \alpha z \qquad \text{with} \qquad \alpha^6 = \frac{2mA}{\hbar^2} \tag{11}$$

$$\lambda = \frac{2mE}{\hbar^2\alpha^2} = E\left(\frac{2m}{\hbar^2}\right)^{2/3}(A)^{-1/3} \tag{12}$$

It can be shown that the period of motion for corresponding classical particle with $V(x) = Ax^4$ is given by [3,4]

$$\tau = \frac{1}{2}\sqrt{\frac{2\pi m}{E}}\left(\frac{E}{A}\right)^{1/4}\frac{\Gamma(1/4)}{\Gamma(3/4)} \tag{13}$$

With $[\Psi(z) = \Psi(x/\alpha) = \psi(x)]$, Eq. (10) becomes

$$\frac{d^2\psi(x)}{dx^2} + (\lambda - x^4)\psi(x) = 0 \tag{14}$$

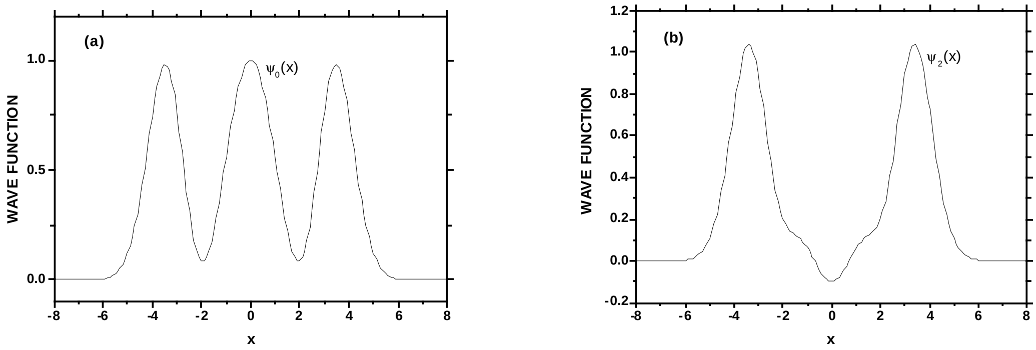
This is Eq. (3) with $\lambda = 2n+1$. Hence for even n

$$\psi_n(x) = Ke^{-x^2/2}\left\{H_n(x) + a_0 x^4\left[-\frac{2!}{4!} + \frac{1}{6!}\left(4! - \frac{4!}{2!}2(-n) - 2^2(4-n)\right)x^2 + \cdots\right]\right\} \tag{15}$$

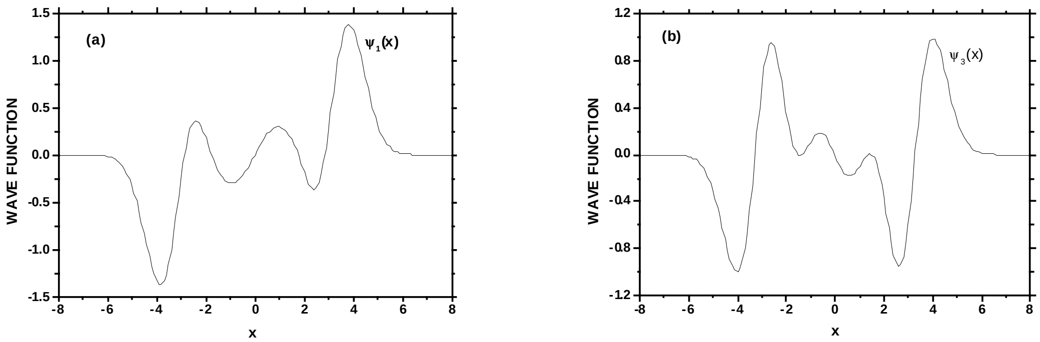
And for odd n

$$\psi_n(x) = Ke^{-x^2/2}\left\{H_n(x) + a_0 x^5\left[-\frac{3!}{5!} + \frac{1}{7!}\left(5! - \frac{5!}{3!}2(1-n) - 3!\times 2(5-n)\right)x^2 + \cdots\right]\right\} \tag{16}$$

The quantum mechanical anharmonic oscillator wave functions (ψ_0, ψ_2 and ψ_1, ψ_3)



Figures 1(a), 1(b): The quantum mechanical anharmonic oscillator wave functions ψ_0 and ψ_2 respectively.



Figures 2(a), 2(b): The quantum mechanical anharmonic oscillator wave functions ψ_1 and ψ_3 respectively.

from Eqs, [15-16] are plotted in Figs. 1 (a), (b) and Figs. 2(a), (b) respectively. In these figures up to five terms in the brackets of Eqs. [15-16] have been included.

Dictating the boundary conditions of the quantum mechanical system, $\lim_{z\to\pm\infty}\Psi(z)=0$ result that n must be an integer. By using Eqs. [12-13] and noting that $\Gamma(1/4)=4\times(\frac{1}{4})!=4$ and $\Gamma(3/4)=\pi\sqrt{2}/4$, energy E becomes

$$E_n=\left(\frac{\lambda}{4}\right)^{3/4}\frac{\Gamma(1/4)}{\sqrt{2\pi}\Gamma(3/4)}\hbar\omega=\left(2n+1\right)^{3/4}\frac{4}{\pi\sqrt{2\pi}}\hbar\omega \tag{17}$$

There is a minimum energy (zero point energy) that is

$$E_0=\frac{4}{\pi\sqrt{2\pi}}\hbar\omega=0.5079\hbar\omega\cong\frac{1}{2}\hbar\omega \tag{18}$$

$$E_1=2.28E_0$$

$$E_2=3.343E_0$$

$$E_3=4.3E_0$$

It is seen that for very large n (at the top of the well) this is ended up with squeezable energy levels, but for small n particularly at the bottom of the well (for E_0 and E_1) we have maximum width in them.

Conclusion

To conclude the Schrödinger wave equation of quantum mechanical anharmonic oscillator with an energy potential of the fourth power of x has been analytically solved. It is shown that the corresponding wave functions differ by a power series of x as compared to that of quantum mechanical simple harmonic oscillator. It is also demonstrated that the corresponding energy levels are wider at the bottom and become more squeezable at the top of the well, although the zero point energy is confirmed.

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