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Excited-State Energy Eigenvalue Evaluation of the Quantum Mechanical Potential $V(x) = \frac{1}{2}m\omega^2x^2 + \mu x^3$ via Numerical Shooting Method

Nonglux Sriboonrueang[1a], Sanit Suwanwong[1b] and Artit Hutem[1c*]

[1]Physics Division, Faculty of Science and Technology, Phetchabun Rajabhat University, Phetchabun, Thailand 67000

[a]koabza10@gmail.com, [b]sanit.suw@gmail.com, [c]magoohootem@yahoo.com
* Corresponding author. E-mail: magoohootem@yahoo.com,
Fax: 056-717-123, Mobile: 086-9909536

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Abstract. The paper deals with eigenvalues excited-state energy eigenvalues and wave-function of a particle under harmonics oscillator asymmetric potential using numerical shooting method. The numerical shooting method is generally regarded as one of the most efficient methods that give very accurate results because it integrates the Schrodinger equation directly, though in the numerical sense. If the value of parameter μ is small the energy eigenvalues of single particle will large and the parameter μ large the energy eigenvalues of single particle will small.

Introduction

Most problems encountered in quantum mechanics cannot be solved exactly. Exact solutions of the Schrodinger equation exist only for a few idealized systems. To solve general problems, one must resort to approximation methods. A variety of such methods have been developed, and each has its own area of applicability. There exist several means to study them, e.g. Wentzel-Kramers-Brillouin [1], perturbation theory[2], the quasilinearization method[3], the variational method, function analysis[3], the eigenvalue moment method[4], the analytical transfer matrix method [5-7] and numerical shooting method[8-9]. In this paper we consider approximation methods that deal with stationary states corresponding to time-independent Hamiltonian. To study problem of stationary states, we focus on one approximation method: numerical shooting method useful evaluate wave-function and energy eigenvalue of a particle around of attraction by the harmonics oscillator with μx^3 potential.

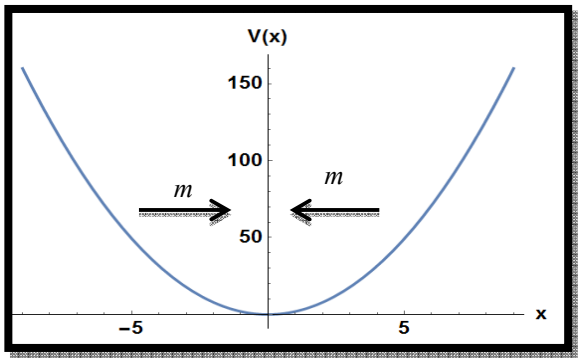


Fig. 1 The harmonics oscillator potential is perturbed by μx^3

In Section 2, we representation of the evaluation of the energy eigenvalue and wave function of particle bound in the $V(x) = \frac{1}{2}m\omega^2x^2 + \mu x^3$ by the numerical shooting method. In Section 3, we make a presentation of numerical and results for energy eigenvalue of a single particle in the potential. The conclusions are given in Section 4.

Schrodinger Equation in Finite Difference formula for $V(x) = \frac{1}{2}m\omega^2x^2 + \mu x^3$

We consider a particle of mass μ moving on the x-axis in a time-independent potential V(x). The time-independent Schrodinger equation corresponding to this one-dimensional motion is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + \left(\frac{1}{2}m\omega^2x^2 + \mu x^3\right)\psi_n(x) = E_n\psi_n(x). \tag{1}$$

Suppose a particle is bound state to around of attraction by the harmonics oscillator μx^3 (see Fig.1). $V(x) = \frac{1}{2}m\omega^2x^2 + \mu x^3$, where μ are constants (μ is real and positive). Substituting potential into eq.(1), and we obtain The one approach we use is the numerical shooting method. To simplify the arithmetic involved in the shooting solution, we define some new dimensionless variables. The position variable *x* is replaced with the dimensionless variable *y*:

$$\frac{d^2\psi_n(y)}{dy^2} + \left(\varepsilon - y^2 - 2\mu y^3\right)\psi_n(y) = 0 \tag{2}$$

We can find the numerical solution eq.(2) by dividing *y* into many small segments, each of Δy in length. The second derivative for the first term of eq.(2) can be approximated in finite difference form as follows

$$\frac{d^2\psi_n(x)}{dy^2} \approx \frac{\psi_{i+1} + \psi_{i+1} - 2\psi_i}{(\Delta y)^2} \tag{3}$$

We can obtain the form of the Schrodinger equation in term of finite difference by substituting eq.(3) into eq.(2), we get

$$\psi_{i+1} = 2\psi_i - \psi_{i-1} - (\Delta y)^2\left(\varepsilon - y^2 - 2\mu y^3\right)\psi_i \tag{4}$$

We construe the new variable for using in calculating the ground-state and excited-state energy eigenvalue, wave-function of $V(x) = \frac{1}{2}m\omega^2x^2 + \mu x^3$.

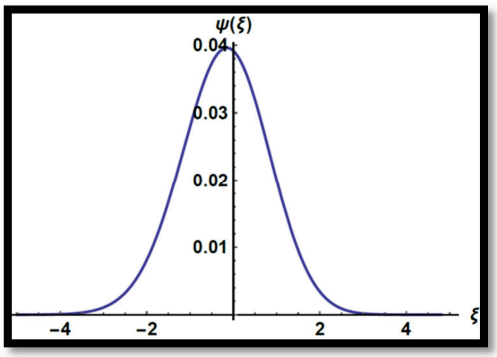
Numerical and Result

We construe the new variable for using in calculating the ground-state and excited-state energy eigenvalue(En), wave-function of the harmonics oscillator asymmetric potential.

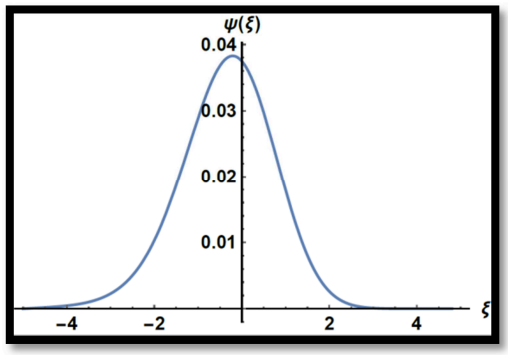
1. y*min* is the start position in the analysis range.
2. y*max* is the ultimate position in the analysis range.
3. y is any position in the analysis range.
4. *nn* is a number of very small bars in the analysis range.
5. Δy is the length of very small bars so that

For the beginning of the numerical shooting method, we need to input parameters *ymin(ymax)*, and Eq. (4) into mathematica program. Next, two initial wave functions are determinate by following two initial conditions as *(i)* $\psi_{(1)} = 0$ is the fixed position and *(ii)* $d\psi / dy = 1$ is the slope of position y1 and *y*2. So we present of wave-functions and energy eigenvalue.

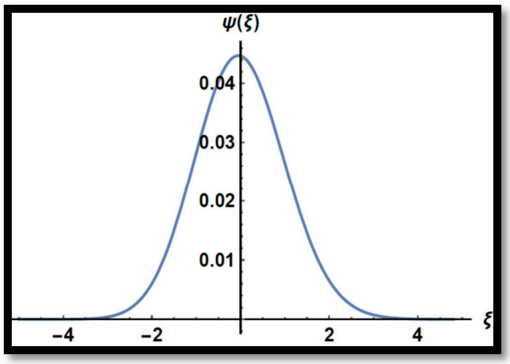
Case 1 ground-state energy $n = 0$



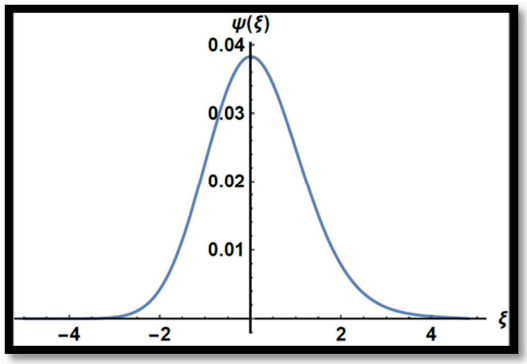
$(a)\varepsilon = 0.99232112,\ \mu = 0.05$



$(b)\varepsilon = 0.96808796,\ \mu = 0.1$



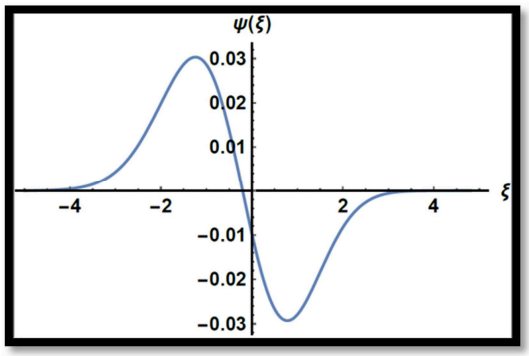
$(c)\varepsilon = 0.99232111,\ \mu = -0.05$



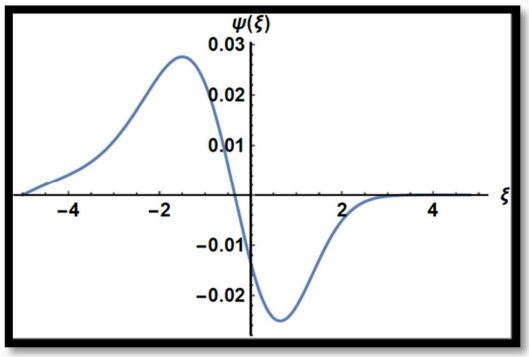
$(d)\varepsilon = 0.96808323,\ \mu = -0.1$

Fig. 2 Schematic representation of the wave-function for ground-state energy (n=0).

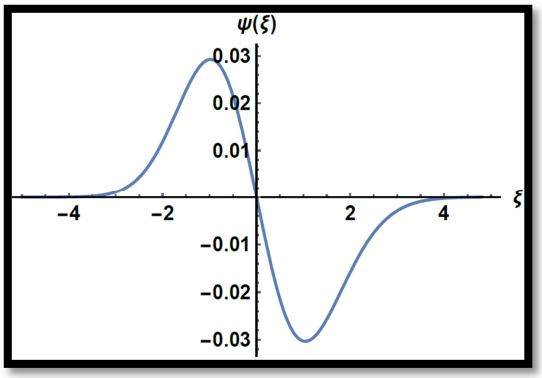
Case 2 excited-state energy $n = 1$



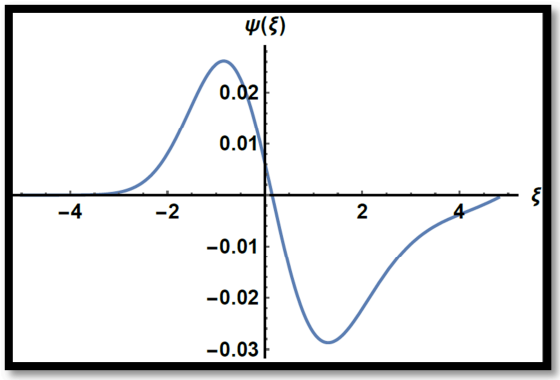
$(a)\varepsilon = 2.95023628,\ \mu = 0.05$



$(b)\varepsilon = 2.75536842,\ \mu = 0.1$



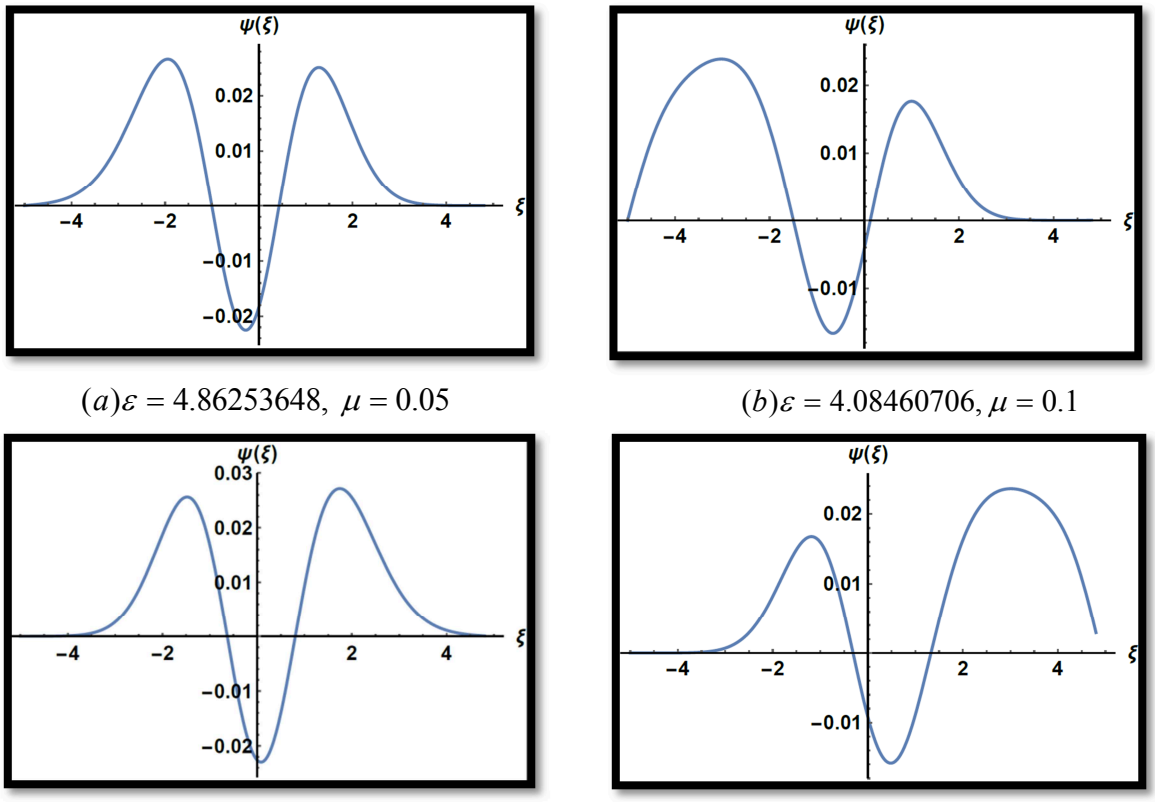
$(c)\varepsilon = 2.95023552,\ \mu = -0.05$



$(d)\varepsilon = 2.75429170,\ \mu = -0.1$

Fig.3 Schematic representation of the wave-function for excited-state energy (n=1)

Case 3 excited-state energy $n = 2$



$(a)\varepsilon = 4.86253648,\ \mu = 0.05$ $(b)\varepsilon = 4.08460706, \mu = 0.1$

$(c)\varepsilon = 4.86251359, \mu = -0.05$ $(d)\varepsilon = 4.03814617, \mu = -0.1$

Fig. 4 Schematic representation of the wave-function for excited-state energy (n=2)

Conclusion

Shrinkage and spreading of the wave function is controlled by parameter μ.

The wave-functions has μ defects (density fluctuation). If the value of parameter μ is small the energy eigenvalues of single particle will large and the parameter μ large the energy eigenvalues of single particle will small.

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