Airy function approach and Numerov method to study the anharmonic oscillator potentials $V(x) = Ax^{2\alpha} + Bx^2$

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Airy function approach and Numerov method to study the anharmonic oscillator potentials $V(x) = Ax^{2\alpha} + Bx^2$

N. Al Sdran[1,2] and F. Maiz[1,3,a]
[1]*King Khalid University, Faculty of Science, Physics Department P.O. Box 9004 Abha, Saudi Arabia*
[2]*Najran University, Faculty of Sciences and Arts, Najran, Saudi Arabia*
[3]*Thermal Process Laboratory Research and Technologies Centre of Energy, BP 95, 2050 Hammam-lif, Tunisia*

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The numerical solutions of the time independent Schrödinger equation of different one-dimensional potentials forms are sometime achieved by the asymptotic iteration method. Its importance appears, for example, on its efficiency to describe vibrational system in quantum mechanics. In this paper, the Airy function approach and the Numerov method have been used and presented to study the oscillator anharmonic potential $V(x) = Ax^{2\alpha} + Bx^2$, $(A>0, B<0)$, with $(\alpha=2)$ for quadratic, $(\alpha=3)$ for sextic and $(\alpha=4)$ for octic anharmonic oscillators. The Airy function approach is based on the replacement of the real potential V(x) by a piecewise-linear potential v(x), while, the Numerov method is based on the discretization of the wave function on the x-axis. The first energies levels have been calculated and the wave functions for the sextic system have been evaluated. These specific values are unlimited by the magnitude of A, B and α. It's found that the obtained results are in good agreement with the previous results obtained by the asymptotic iteration method for $\alpha=3$. [http://dx.doi.org/10.1063/1.4954923]

I. INTRODUCTION

The description of vibratory system in quantum mechanics is very important for young researchers and scientists and also to have a deep understanding for its future applications. Some methods have been established to determine with precision the energy spectra of many anharmonic oscillators.[1] They have been carried out using the Hill determinant,[2,3] the coupled cluster method,[4,5] the Bargmann representation,[6,7] the variational-perturbation expansion and other approaches.[8–13] Using the double exponential Sinc collocation method, Gaudreau *et al.*[14] evaluated the energy eigenvalues of anharmonic oscillators. For bounded anharmonic oscillators, Alhendi *et al.*[15] used a power-series expansion and Fernández[16] applied the Riccati–Padé method, to calculate their accurate eigenvalues. A variant of approximate methods and numerical techniques has recently been developed,[17–24] to calculate with high precision, the spectrum of one-dimensional symmetric anharmonic oscillators. Barakat[25] used the asymptotic iteration method (AIM) to calculate the eigen-energies for the anharmonic oscillator potentials $V(x) = Ax^{2\alpha} + Bx^2$, he introduced an adjustable parameter β to improve the AIM rate of convergence. However, the choice of the adjustment parameters is not usually simple. F. Maiz and S. AlFaify[26] have applied the airy function approach to study the anharmonic oscillator potentials $V(x) = x^8 \pm x^2$.

In this paper, using both the Airy Function Approach (AFA) and the Numerov Method (NM), we study the anharmonic oscillator potentials $V(x) = Ax^{2\alpha} + Bx^2$. This paper is organized as follows. In Sect. II, we recall these two methods. In Sect.III, we study quadratic, sextic and octic

[a]corresponding author: tel: +966505331750, fax: +96672418319,email: fethimaiz@gmail.com

anharmonic oscillator potentials $V(x) = Ax^{2\alpha} + Bx^2$ for α=2, 3 and 4, we sketch the variations of the normalized waves functions associated to the first six states of energies as a function of the position, and we compare our results with the previous published ones.

II. FORMULATION

Solving the one-dimensional time-independent Schrödinger equation is an essential and primary step in order to calculate the energy eigenvalues for anharmonic oscillator potential, (without loss of generality, we assume throughout this paper, that $\hbar^2 = 2m$ where $\hbar$ is the Planck constant and m the particle mass.):

$$\frac{d^2\Psi(x)}{dx^2} + (E - V(x))\Psi(x) = 0 \tag{1}$$

Where $\Psi(x)$ is the wave function, $V(x)$ is the potential energy and E the energy system. According to Barakat[25] the solution of Schrödinger's equation can be written as: $\Psi_n(x) = f_n(x)e^{-\beta\frac{x^2}{2}}$.

Where β is an adjustable parameter has been introduced to improve the rate of convergence of the objective. However, it is clear that the choice of the best parameter to obtain quickly the good results without violating the principle of the method is not obvious. To avoid this difficulty, the airy function approach and the Numerov method have been used to study the anharmonic oscillator potentials $V(x) = Ax^{2\alpha} + Bx^2$, and results will been compared to those achieved by the asymptotic iteration method.[25]

A. Airy function approach

The potential energy function $V(x)$ is a continuous function of the one space variable x. In order to solve Eq. (1), $V(x)$ is approached with a piecewise linear potential function $\vartheta(x)$, by dividing the x-axis into (n+1) intervals $I_i = [x_i, x_{i+1}]$, where $i = 0, 1, 2, \ldots\ldots n$.

For $x_i \le x \le x_{i+1}$ the linear potential function is given by the expression: $\vartheta(x) = V(x_i) + s_i x$, where x denotes the distance from the interface x_i and s_i the slop of the linear potential: $s_i = (V(x_{i+1}) - V(x_i))/(x_{i+1} - x_i)$, the interval's width is $h_i = (x_{i+1} - x_i)$. For large value of n the potential energy function and the approached linear one are closed up. Fig. 1 shows the real potential and the piecewise linear potential one, they go well together on all the x-axis, except in the intervals 1 and i.

The solution of the Schrödinger equation (1) across the interval I_i $\Psi_i(x)$ can be expressed as a linear combination of two functions ϕ and φ as:

$$\Psi_i(x) = X_i\phi_i(z) + Y_i\varphi_i(z) \tag{2}$$

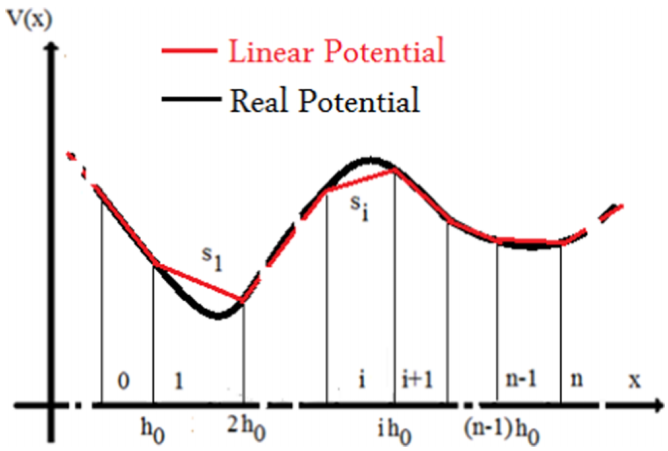

FIG. 1. Profiles of the real potential V(x) and the linear one v(x).

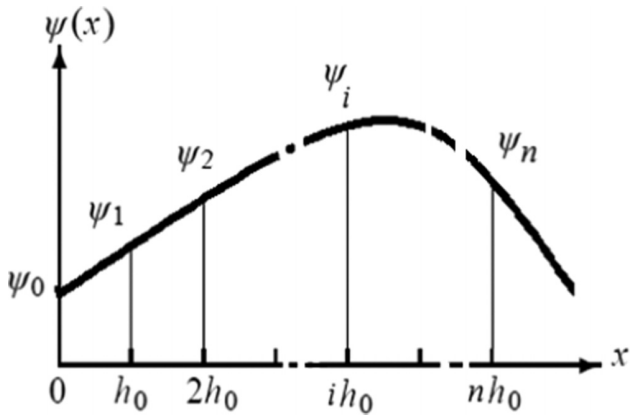

FIG. 2. Discretization of the wave function.

Where X_i and Y_i are constants and:

- For linear potential ($s_i \neq 0$) : $\phi_i(z) = Ai(z)$ and $\varphi_i(z) = Bi(z)$ where Ai and Bi are the Airy functions, and $z = (V_i - e + s_i x)/s_i^{2/3}$.
- For constant potential ($s_i = 0$): $\phi_i(z) = \exp(-z)$ and $\varphi_i(z) = \exp(z)$ where $z = k_i x$, and $k_i = \sqrt{V_i - e}$ the wave vector modulus.

At each interface x_i, the wave function and its first derivative are continuous. Analytically, this interprets into:

$$\Psi_i(x_i) = \Psi_{i+1}(x_i) \qquad \text{and} \qquad \Psi_i'(x_i) = \Psi_{i+1}'(x_i) \tag{3}$$

Where the prime denotes the first derivative with respect to x.

Equations (2) and (3) lead to the following equation known as the energy quantification condition:

$$B(E) = Q_n = 0 \tag{4}$$

To determine Q_n, we use the following progressions:

$$Q_i = W(\varphi_{(i-1)}(h_{(i-1)}); \phi_{(i)}(0))Q_{i-1} - W(\phi_{(i-1)}(h_{(i-1)}); \phi_{(i)}(0))P_{i-1}$$
$$P_i = W(\varphi_{(i-1)}(h_{(i-1)}); \varphi_{(i)}(0))Q_{i-1} - W(\phi_{(i-1)}(h_{(i-1)}); \varphi_{(i)}(0))P_{i-1}$$
$$Q_1 = W(\phi_{(1)}(0); \phi_{(0)}(h_{(0)}))P_1 = W(\varphi_{(1)}(0); \phi_{(0)}(h_{(0)}))$$

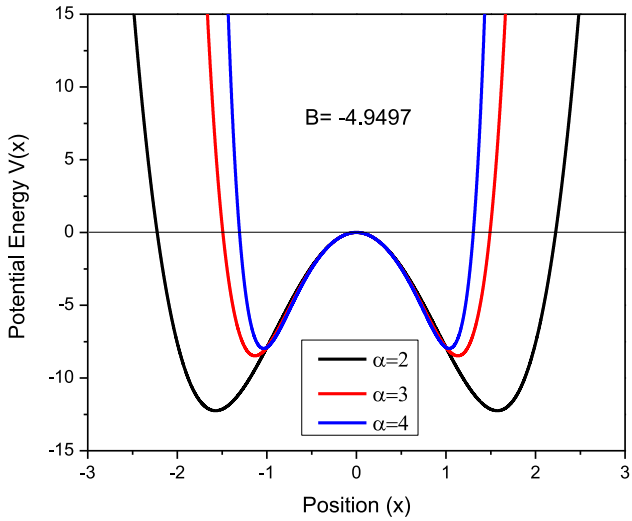

FIG. 3. Variation of the potential $V(x) = Ax^{2\alpha} + Bx^2$ as a function of the position for A=1, B=-4.9497 and α=2, 3 and 4.

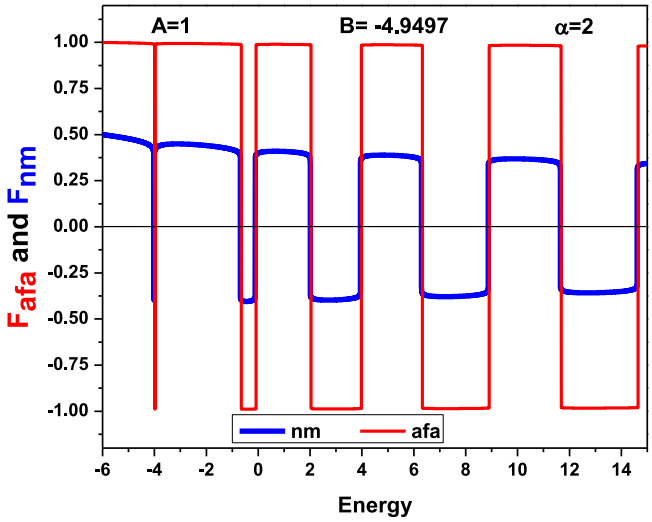

FIG. 4. Variations of the functions $F_{afa}(E)$ and $F_{nm}(E)$ as a function of energy for the potential $V(x) = Ax^{2\alpha} + Bx^2$ with A=1, B=-4.9497 and α=2.

and for each two functions $f_{(i)}$ and $g_{(j)}$:

$$W(f_{(i)}(h_{(i)}); g_{(j)}(h_{(j)})) = f_{(i)}(h_{(i)})g'_{(j)}(h_{(j)}) - f'_{(i)}(h_{(i)})g_{(j)}(h_{(j)}).,$$

We note that for each quantity x: $x_{(i)} = x_i$

The above expressions can be approved in the general case by the recurrence method.[27–29] The energy levels are obtained by the energy values for which the curve of B(E) meets the energy axis. Because of the large values of the function B(E) and its many variations, the graphical search of its roots does not necessarily. Hence, it is changed by the function $F_{afa}(E)$ defined as:

$$F_{afa}(E) = \text{signum}(B(E))\frac{\log(|B(E)|)}{\log(|B(E)|_{max})} \quad (5)$$

where the signum function computes the sign of the argument [if x≠0 then signum(x)= x/abs(x), and signum(0)=0]. The energy levels are indicated by vertical red segments perpendicular to the

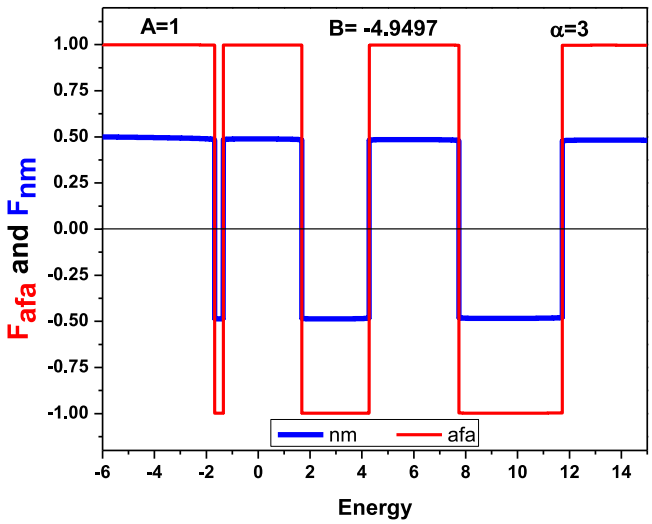

FIG. 5. Variations of the functions $F_{afa}(E)$ and $F_{nm}(E)$ as a function of energy for the potential $V(x) = Ax^{2\alpha} + Bx^2$ with A=1, B=-4.9497 and α=3.

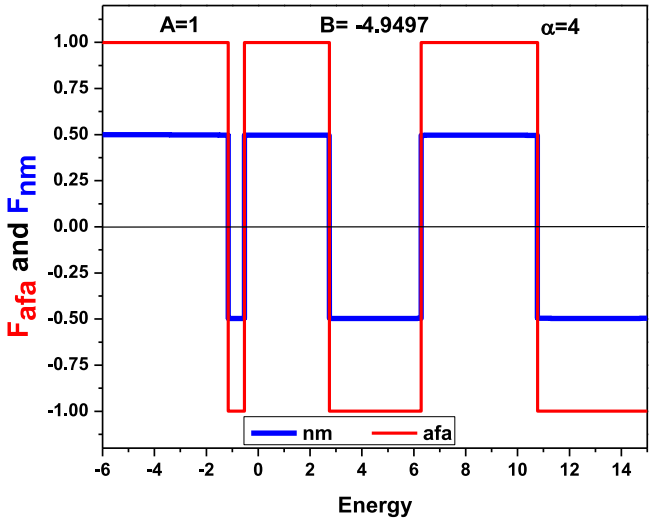

FIG. 6. Variations of the functions $F_{afa}(E)$ and $F_{nm}(E)$ as a function of energy for the potential $V(x) = Ax^{2\alpha} + Bx^2$ with A=1, B=-4.9497 and α=4.

energy axis which constitute the curve of the function $F_{afa}(E)$. In this case, the energy levels are with a great precision, they were obtained by using n around 4000.

B. Numerov method

In order to find the energy eigenvalues, we need to be able to integrate Eq. (1) with respect to x, for a given value of E, starting at $x = x_0$, i.e, with some specified values for $x = x_0$ and $x = x_1 = x_0 + h$, where h is the step interval. Using the notation $x_n = x_0 + nh$ and $\Psi_n = \Psi(x_n)$, we have to solve for $\Psi_2, \Psi_3, \ldots\ldots$, given Ψ_0 and Ψ_1 (see Figure 2).

A Taylor series for $\Psi(x + h)$ gives

$$\Psi(x + h) = \Psi(x) + h\Psi'(x) + h^2\Psi^{(2)}(x)/2 + h^3\Psi^{(3)}(x)/6 + h^4\Psi^{(4)}(x)/24 + \ldots\ldots \quad (6)$$

By adding this to the series for $\Psi(x - h)$ all the odd powers of h vanish:

$$\Psi(x + h) + \Psi(x - h) = 2\Psi(x) + h^2\Psi^{(2)}(x)/2 + h^4\Psi^{(4)}(x)/12 + O(h^6) \quad (7)$$

TABLE I. Obtained energy eigenvalues by the Airy Function Approach and the Numerov Method for α=2,3 and 4, and the Asymptotic Iteration Method for α=3, and A=1, B=-4.9497.

	A=1, B=-4.9497						
	E (α=2)		E (α=3)			E (α=4)	
n	AFA	NM	AIM	AFA	NM	AFA	NM
0	-4.0235	-4,0245	**−1.6818**	-1.6805	-1,6815	-1.1535	-1,1545
1	-4.0065	-4,0065	**-**	-1.3465	-1,3475	-0.5325	-0,5335
2	-0.6905	-0,6905	**1.6818**	1.6825	1,6815	2.7435	2,7415
3	-0.1155	-0,1155	-	4.2805	4,2795	6.2855	6,2825
4	2.0045	2,0045	-	7.7375	7,7355	10.7685	10,7655
5	3.9435	3,9785	-	11.7275	11,7255	-	-
6	6.2975	6,2965	-	-	-	-	-
7	8.8665	8,8655	-	-	-	-	-
8	11.6465	11,6465	-	-	-	-	-
9	14.6095	14,6085	-	-	-	-	-

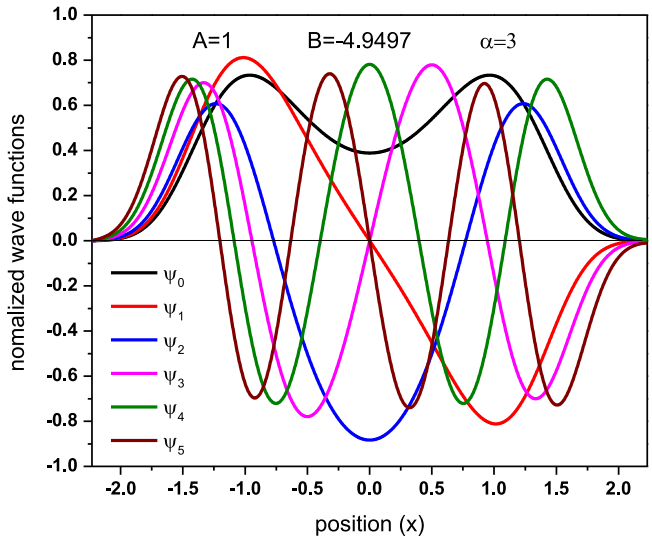

FIG. 7. Normalized wave functions curves as function of position for the six first states and the potential $V(x) = Ax^{2\alpha} + Bx^2$ with A=1, B=-4.9497 and α=3.

We can therefore write the second derivative which occurs in the Schrödinger equation, Eq. (1), as

$$\Psi^{(2)}(x) = \frac{\Psi(x+h) + \Psi(x-h) - 2\Psi(x)}{h^2} - h^4\Psi^{(4)}(x)/12 + O(h^4) \tag{8}$$

We would like to evaluate the term involving the 4th derivative. To do so, we act on Eq. (1) with $(1 + (h^2/12)d^2/dx^2)$, which gives

$$\Psi^{(2)}(x) + h^4\Psi^{(4)}(x)/12 + k^2(x)\Psi(x) + h^2/12d^2/dx^2[k^2(x)\Psi(x)] = 0 \tag{9}$$

Substituting for $\Psi^{(2)}(x) + h^4\Psi^{(4)}(x)/12$ from Eq. (8) into Eq. (9) leads to

$$\Psi(x+h) + \Psi(x-h) - 2\Psi(x) + h^2k^2(x)\Psi(x) + h^2/12d^2/dx^2[k^2(x)\Psi(x)] + O(h^6) = 0 \tag{10}$$

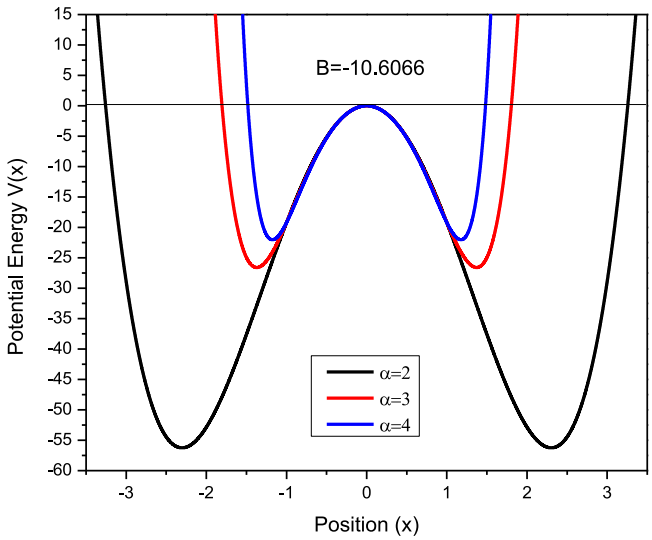

FIG. 8. Variation of the potential $V(x) = Ax^{2\alpha} + Bx^2$ as function of the position for A=1, B=-10.6066 and α=2, 3 and 4.

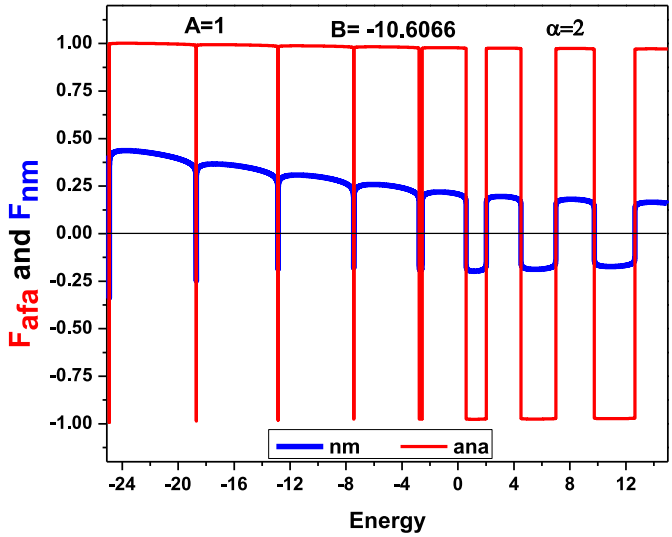

FIG. 9. variations of the functions $F_{afa}(E)$ and $F_{nm}(E)$ as a function of energy for the potential $V(x) = Ax^{2\alpha} + Bx^2$ with A=1, B=-10.6066 and α=2.

Using an elementary deference formula, we evaluate $d^2/dx^2[k^2(x)\Psi(x)]$

$$d^2/dx^2[k^2(x)\Psi(x)] \cong \frac{k^2(x+h)\Psi(x+h) + k^2(x-h)\Psi(x-h) - 2k^2(x)\Psi(x)}{h^2} \tag{11}$$

Substituting Eq. (11) into Eq. (10) and rearranging, we get the Numerov algorithm for one time step:

$$\Psi(x+h) = \frac{2(1 - 5h^2k^2(x)/12)\Psi(x) - (1 + h^2k^2(x-h)/12)\Psi(x-h)}{(1 + h^2k^2(x+h)/12)} + O(h^6) \tag{12}$$

Setting $x = x_n = x_0 + nh$, and defining $k_n \equiv k(x_n)$, this can be written more precisely as:

$$\Psi_{n+1} = \frac{2(1 - 5h^2k_n^2/12)\Psi_n - (1 + h^2k_{n-1}^2/12)\Psi_{n-1}}{(1 + h^2k_{n+1}^2/12)} \tag{13}$$

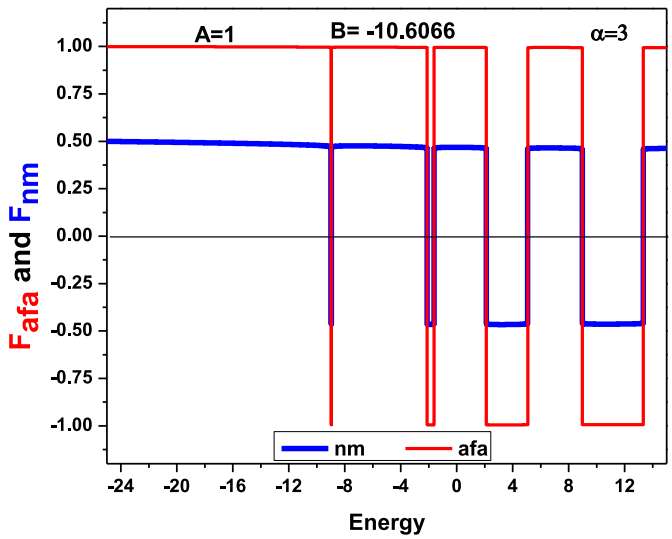

FIG. 10. Variations of the functions $F_{afa}(E)$ and $F_{nm}(E)$ as a function of energy for the potential $V(x) = Ax^{2\alpha} + Bx^2$ with A=1, B=-10.6066 and α=3.

The Numerov method, Eq. (13), can be used to determine Ψ_n for n=2,3,4,...., given two initial values, Ψ_0 and Ψ_1. Equation (13) leads to the following equation known as the energy quantification condition: $\Psi_n = 0$. The energy levels are obtained by the energy values for which the curve of $\Psi_n(E)$ meets the energy axis. For a good research of eigenenergies, we use the following expression similar to the AFA ones:

$$F_{nm}(E) = \frac{1}{2}\text{signum}(\Psi_n(E))\frac{\log(|\Psi_n(E)|)}{\log(|\Psi_n(E)|_{max})} \quad (14)$$

In order to differentiate the curves of $F_{afa}(E)$ (solid red line) and $F_{nm}(E)$ (solid blue line), the signum function is divided by 2. The energy levels are indicated by vertical blue segments perpendicular to the energy axis. In this case, the energy levels are with high accuracy, they were made by n=5000.

III. APPLICATIONS

As applications, the anharmonic oscillator potential $V(x) = Ax^{2\alpha} + Bx^2$ was studied for three values of α (2, 3 and 4) and two values of (B =-4.9497 and -10.6066) and A=1 (A and B are real constants and α is the power factor).

A. Study of the potential $V(x) = Ax^{2\alpha}$-4.9497 x^2

Figure 3 shows the variations of the potential V(x) as a function of the position x. It is the case of double quantum wells, we observe that the wells deep's and the distance between each double wells increase with the power factor, by against the interaction between each double wells decrease.

Figures (4-6) show the variations of the functions $F_{afa}(E)$ and $F_{nm}(E)$ as a function of energy for the coefficients for A=1, B=-4.9497 and the power factor α=2, 3 and 4. These two functions meet the energy axis simultaneously and give practically the same energy eigenvalues. For the value of energy of -4 and α=2, we found that the two curves pass through the energy axis in the two directions rapidly; this means that we have a double degenerated state. This is due to the quantum tunneling, in fact for small values of the power factor α the two wells are the deepest and the tunnel effect appears.

Table I displays the energy eigenvalues obtained by the airy function approach and the Numerov method. These two methods give the same results and closed to those already calculated by the AIM.[25] It is noteworthy that the relative error is less than 10^{-4}.

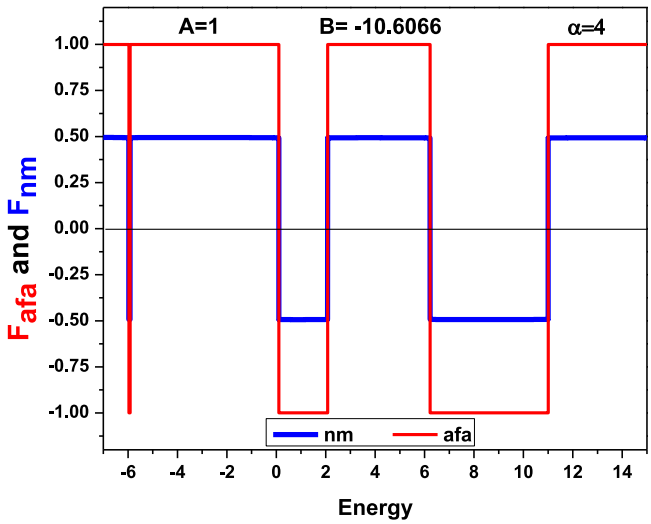

FIG. 11. Variations of the functions $F_{afa}(E)$ and $F_{nm}(E)$ as a function of energy for the potential $V(x) = Ax^{2\alpha} + Bx^2$ with A=1, B=-10.6066 and α=4.

TABLE II. Obtained energy eigenvalues by the Airy Function Approach and the Numerov Method for α=2,3 and 4, and the Asymptotic Iteration Method for α=3, and A=1, B=-10.6066.

	A=1, B=-10.6066						
	E (α=2)		E (α=3)			E (α=4)	
N	AFA	NM	AIM	AFA	NM	AFA	NM
0	-24.9185	-24,9185	**−8.9651**	-8.9625	-8,9655	-5.9645	-5,9675
1	-24.9165	-24,9165	-	-8.9585	-8,9605	-5.9145	-5,9175
2	-18.7115	-18,7115	**−2.1164**	-2.1155	-2,1165	0.1055	0,1045
3	-18.7095	-18,7095	-	-1.6255	-1,6265	2.0785	2,0755
4	-12.8615	-12,8615	-	2.1175	2,1165	6.2245	6,2225
5	-12.8595	-12,8595	-	5.0715	5,0695	11.0035	10,9985
6	-7.4525	-7,4555	-	8.9675	8,9655	-	-
7	-7.4435	-7,4475	-	13.3345	13,3315	-	-
8	-2.7785	-2,7805	-	-	-	-	-
9	-2.5585	-2,5625	-	-	-	-	-
10	0.5815	0,5795	-	-	-	-	-
11	2.0235	2,0215	-	-	-	-	-

Figure 7 shows the variations of the normalized wave functions curves as function of position for the six first states and the potential $V(x) = Ax^{2\alpha} + Bx^2$ with A=1, B=-4.9497 and α=3. We start by the AFA approach method to calculate the energy levels values, and then we use the Numerov method to search and verify our results and calculate the normalized wave function. We observe three even functions Ψ_0,Ψ_2, and Ψ_4 and three odd functions Ψ_1,Ψ_3, and Ψ_5. Unlike the case of the harmonic oscillator Ψ_0 doesn't reach its maximum value at zero point. All functions vanish for $|x| \geq 2.3$.

B. Study of the potential $V(x) = Ax^{2\alpha}$-10.6066 x^2

Figure 8 shows the variation of the potential V(x) as a function of the position x. In this case, the maximum depth of the wells is approximately 56.39.

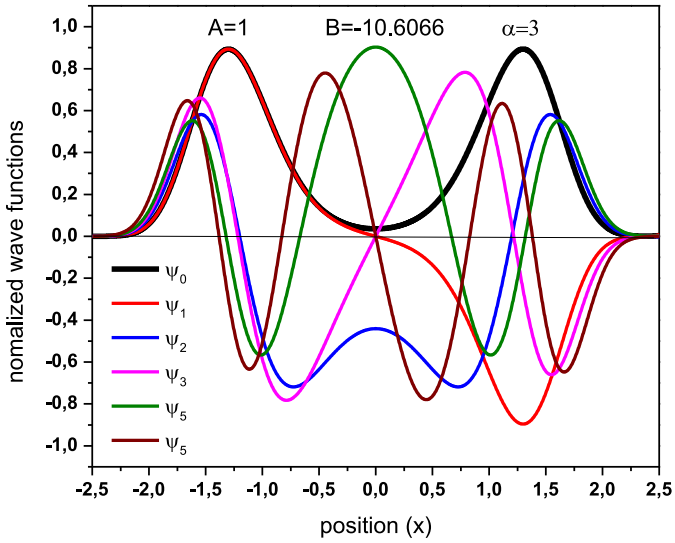

FIG. 12. Normalized wave functions curves as function of position for the six first states and the potential $V(x) = Ax^{2\alpha} + Bx^2$ with A=1, B=-10.6066 and α=3.

Figures (9-11) show the variations of the functions $F_{afa}(E)$ and $F_{nm}(E)$ as a function of energy for the coefficients for A=1, B=-10.6066 and the power factor α=2, 3 and 4. Table II displays the energy eigenvalues obtained by these numerical methods and those already calculated by the asymptotic iteration method.[25] In this case there are five states doubly degenerated (-24.9, -18.7, -12.86, -7.4, and -2.76) for α=2, and only one for the other values of α.

Table II. gives the energy eigenvalues obtained by the airy function approach and the Numerov method and those already calculated by Ref. 25. The results are closed and the relative error is less than 10^{-4}.

Figure 12 shows the variations of the normalized wave functions curves as function of position for the six first states and the potential $V(x) = Ax^{2\alpha} + Bx^2$ with A=1, B=-10.6066 and α=3. We observe three even functions Ψ_0, Ψ_2, and Ψ_4 and three odd functions Ψ_1, Ψ_3, and Ψ_5 and pass through zero. Unlike the case of the harmonic oscillator Ψ_0 doesn't reach its maximum value at zero point. All functions vanish for $|x| \geq 2.5$.

IV. CONCLUSION

The airy function approach and the Numerov method were successfully used to solve anharmonic oscillator problems. In the first method, the real potential V(x) was approximated by a piecewise linear potential v(x). Then, the Schrödinger's equation solution was found as a combination of Airy functions or plane waves, the continuity conditions of each solution and their first derivatives through interfaces, lead to the energy quantification condition. For the second method, we start by the discretization of the wave function and assume that Ψ_0 and Ψ_1 are closed to zero, then, the energy levels have been deduced by the energy value for which the wave function vanishes. Because of the large values of the energy quantification conditions and their multiple abrupt changes, we have chosen to write it as a simpler form and which allow a good visibility of their roots. The energy levels are set by vertical segments to the energy axis. Using these previous method, we have study the anharmonic oscillator potentials $V(x) = Ax^{2\alpha} + Bx^2$ for three values of α (2, 3 and 4), two values of (B =-4.9497 and -10.6066) and A=1. We start by the first method to known the energy levels values, then we use to second one to search and verify our results and calculate the normalized wave function. Archived results are not only with high degree of accuracy but also both satisfactory and not computationally complicated, and agree very well with the previous ones for α=3.

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