Approximate solutions of Schroedinger equation

Konstantinos Rafail Revis[1]
[1] *Department of Physics, Aristotle University of Thessaloniki, Thessaloniki* 54124, *Greece*

In this letter our primary goal is to introduce approximate solutions for the energy of the Schroedinger equation (S.E.). Firstly, we are going to work for a particle inside a infinity well, considering a linear and parabolic potential. Even though the problem without the potential can be considered as overused, the solution of the S.E. with a potential, leads to a rather complicated mathematical problem and its solution is going to be provided with two different ways. On one hand, we are going to present the solution with perturbation theory and on the other hand, we are going to use the Wolfram Mathematica© [8] to calculate the approximate solution. Then, we are going to compare the different solutions and assert if it is possible to end up with similar results. In conclusion, we are going to introduce a monomial potential and then the S.E. will be solved using the Frobenius method.

I. INTRODUCTION

A. Frobenius Method

Unfortunately, there is not a general formula to solve a differential equation of the following form:

$$W(x)u''(x) + R(x)u'(x) + T(x)u(x) = 0. \tag{1}$$

A useful approximation method has been developed, if we try to solve an equation of the form (1), at an arbitrary point x_0. It is also helpful to theorize that $x_0 = 0$. According to [4], this method is called Frobenius method and we assume that the solution of (1) can be written as:

$$u(x) = x^k \sum_{n=0}^{\infty} c_n x^n. \tag{2}$$

It is, also, possible to use the following form, if the point we choose is a regular one:

$$u(x) = \sum_{n=0}^{\infty} c_n x^n. \tag{3}$$

Firstly, we have to obtain the following results:

$$u'(x) = \sum_{n=0}^{\infty} n c_n x^{n-1}. \tag{4}$$

and

$$u''(x) = \sum_{n=0}^{\infty} n(n-1) c_n x^{n-2}. \tag{5}$$

After we rearrive equation (1), taking into account the previous assumption and its results, we are able to obtain a polynomial that should equal to zero. Then, hypothesizing that $c_0 \neq 0$, we can obtain one or many possible retroactive equations and then arrive to a result, where all the coefficients are given as a function of c_0 and c_1. It must be denoted that, for the general solution of the equation (1), two arbitrary constants are required. It must be underlined that it is not unusual, that c_1 vanishes.

B. The infinite potential well

We are going to begin our analysis with the well-known infinite potential well. Firstly, let us introduce the time independent and one dimensional S.E. as is given by D. Griffiths in [3]:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + (V(x) - E)\right)\psi(x) = 0, \tag{6}$$

where m is the mass, $V(x)$ is the potential, $\psi(x)$ is the wave function, E is the Energy and $\hbar$ is the reduced Planck constant. In this case, the potential is given by the following equation:

$$V(x) = \begin{cases} 0 & 0 \leq x \leq L \\ \infty & otherwise \end{cases}$$

So, if we start solving the S.E. for $0 \leq x \leq L$, arrive at the following differential equation:

$$\psi''(x) + \frac{2mE}{\hbar^2}\psi = 0, \tag{7}$$

and we are going to work only for $E > 0$. If we set $k^2 = \frac{2mE}{\hbar^2}$ we arrive at:

$$\psi''(x) + k^2\psi = 0 \tag{8}$$

The equation (8) is the well-known equation of the harmonic oscillation and its solution is given as it follows [1]:

$$\psi(x) = A\cos(kx) + B\sin(kx), \tag{9}$$

where A and B are some arbitrary constants, that can be determined thanks to the following boundary conditions:

$$\psi(0) = \psi(L) = 0, \tag{10}$$

so we find that $A = 0$. If we consider $\psi(L) = 0$, there are two options. The first is that $B = 0$ but in this case, the wave function is always zero and the second is that $B\sin kL = 0$. Obviously, the second option has a physical meaning, so we need to solve the following equation:

$$\sin kL = 0 \Rightarrow kL = n\pi, n \in \mathbb{Z}. \tag{11}$$

Recalling that $k^2 = \frac{2mE}{\hbar^2}$ and by combining with (11), we obtain that the possible values of energy are given by the equation:

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}. \tag{12}$$

In order to determine B, we have to take into consideration the normalization of the wave function so:

$$\langle\psi|\psi\rangle = 1 \Rightarrow \int_0^L B^2\sin^2 kx dx = 1 \tag{13}$$

so we, finally, obtain that the wave function is given by the equation:

$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin\frac{n\pi x}{L}. \tag{14}$$

II. POTENTIAL FORM $V(x) = ax + c$ INSIDE THE INFINITE POTENTIAL WELL

We are going to proceed our analysis by introducing the following potential:

$$V(x) = ax + c\ ,\ a > 0 \tag{15}$$

where

$$\mathcal{O}(a) = \mathcal{O}(c). \tag{16}$$

and

$$a, c << 1. \tag{17}$$

We chose that type of potential, with the aforementioned constrains, because the linear is the simplest possible function of x and we are able to build on the obtained results, the following analysis provides. By recalling equation (6), after some simple calculations we obtain that:

$$\psi''(x) - \frac{2m}{\hbar^2}\left(ax + c - E\right)\psi(x) = 0. \tag{18}$$

If we set $A = \frac{2m}{\hbar^2}$, we arrive at the following differential equation:

$$\psi''(x) - A\left(ax + c - E\right)\psi(x) = 0. \tag{19}$$

According to [3], the equation (19) is a form of the Airy differential equation and its solution is the linear combination on the Airy functions $A_i(x)$ and $B_i(x)$, so we finally find the solution is the following:

$$\psi(x) = c_1 A_i\left(\frac{aAx + Ac - AE}{(aA)^{2/3}}\right) + c_3 B_i\left(\frac{aAx + Ac - AE}{(aA)^{2/3}}\right), \tag{20}$$

where c_1 and c_3 are some arbitrary constants, which are going to be calculated thanks to the boundary conditions and the normalization of the wave function. The first boundary condition is $\psi(0) = 0$, so, by starting the calculations, we finally obtain that:

$$c_1 = -\frac{c_3 B_i\left(\frac{Ac-AE}{(aA)^{2/3}}\right)}{A_i\left(\frac{Ac-AE}{(aA)^{2/3}}\right)}. \tag{21}$$

The second boundary condition is $\psi(L) = 0$, but in this case $c_3 = 0$ and $c_1 = 0$ so there is no physical meaning for these results. If bear in mind the normalization of the wave function, we have to solve the following equation:

$$\int_0^L \psi(x)^2\, dx = 1, \tag{22}$$

considering c_3 as the unknown parameter, and after a lot calculations we end up with the following result:

$$c_3 = \left(\frac{q_1 + q_2 + q_3 + q_4 + q_5 + q_6 + q_7 + q_8}{aAA_i\left(\frac{A(c-E)}{(aA)^{2/3}}\right)^2}\right)^{-1/2}, \tag{23}$$

where $q_1, q_2, q_3, q_4, q_5, q_6, q_7$ and q_8 are defined as following:

$$q_1 = A(aL + c - E)B_i\left(\frac{A(c-E)}{(aA)^{2/3}}\right)^2 A_i\left(\frac{A(c-E+aL)}{(aA)^{2/3}}\right)^2 + AcA_i\left(\frac{A(c-E)}{(aA)^{2/3}}\right)^2 B_i\left(\frac{A(c-E+aL)}{(aA)^{2/3}}\right)^2, \tag{24}$$

$$q_2 = -AEA_i\left(\frac{A(c-E)}{(aA)^{2/3}}\right)^2 B_i\left(\frac{A(c-E+aL)}{(aA)^{2/3}}\right)^2, \tag{25}$$

$$q_3 = aALA_i\left(\frac{A(c-E)}{(aA)^{2/3}}\right)^2 B_i\left(\frac{A(c-E+aL)}{(aA)^{2/3}}\right)^2, \tag{26}$$

$$q_4 = -2A(aL + c - E)A_i\left(\frac{A(c-E)}{(aA)^{2/3}}\right) B_i\left(\frac{A(c-E)}{(aA)^{2/3}}\right) A_i\left(\frac{A(c-E+aL)}{(aA)^{2/3}}\right) B_i\left(\frac{A(c-E+aL)}{(aA)^{2/3}}\right), \tag{27}$$

$$q_5 = -(aA)^{2/3}A_i\left(\frac{A(c-E)}{(aA)^{2/3}}\right)^2 B_i'\left(\frac{A(c-E+aL)}{(aA)^{2/3}}\right)^2 - (aA)^{2/3}B_i\left(\frac{A(c-E)}{(aA)^{2/3}}\right)^2 A_i'\left(\frac{A(c-E+aL)}{(aA)^{2/3}}\right)^2, \tag{28}$$

$$q_6 = 2(aA)^{2/3}A_i\left(\frac{A(c-E)}{(aA)^{2/3}}\right) B_i\left(\frac{A(c-E)}{(aA)^{2/3}}\right) A_i'\left(\frac{A(c-E+aL)}{(aA)^{2/3}}\right) B_i'\left(\frac{A(c-E+aL)}{(aA)^{2/3}}\right), \tag{29}$$

$$q_7 = +(aA)^{2/3} A_i \left(\frac{A(c-E)}{(aA)^{2/3}} \right)^2 B_i' \left(\frac{A(c-E)}{(aA)^{2/3}} \right)^2 + (aA)^{2/3} A_i' \left(\frac{A(c-E)}{(aA)^{2/3}} \right)^2 B_i \left(\frac{A(c-E)}{(aA)^{2/3}} \right)^2, \tag{30}$$

$$q_8 = -2(aA)^{2/3} A_i \left(\frac{A(c-E)}{(aA)^{2/3}} \right) A_i' \left(\frac{A(c-E)}{(aA)^{2/3}} \right) B_i \left(\frac{A(c-E)}{(aA)^{2/3}} \right) B_i' \left(\frac{A(c-E)}{(aA)^{2/3}} \right). \tag{31}$$

A textbook solution requires to substitute $x = L$ and solve the equation $\psi(L) = 0$ in order to determine the possible values of E. Obviously, it is impossible to obtain the analytical solution of this equation so we have to find an other way to obtain a sufficient result. It must be underlined that we are able to use approximation formulas for the Airy functions $A_i(x)$ and $B_i(x)$, for $x \to \pm\infty$, which could make the so called textbook solution more possible.

A. Perturbation Theory Approach

According to [3], perturbation theory is a well defined procedure to obtain approximate solutions for a quantum mechanical system, if we introduce perturbation in a well known and solvable system. In section I B, we introduced a solvable system and in section III, we came face to face with a rather complicated mathematical problem. For this approach, it must be underlined that there is no degeneration in the unperturbed problem so the correction of first order is given as it follows [3]:

$$E_n^{(1)} = \left\langle \psi_n^{(0)} \left| V_1(x) \right| \psi_n^{(0)} \right\rangle, \tag{32}$$

where $\psi_n^{(0)}$ is the wave function of the unperturbed problem and $V_1(x)$ is the added perturbation. So first order approximation for the energy of the perturbed problem, is the following:

$$E_n = E_n^{(0)} + E_n^{(1)}, \tag{33}$$

where $E^{(0)}$ is the energy of the unperturbed problem. By bearing in mind the equations (15) and (32) we end up to the following result:

$$E_n^{(1)} = \int_0^L \frac{2(ax+c)\sin^2\left(\frac{\pi n x}{L}\right)}{L} \, dx \Rightarrow \tag{34}$$

$$E_n^{(1)} = \frac{2\pi^2 n^2 (aL + 2c) - 2\pi n \sin(2\pi n)(aL + c) - aL\cos(2\pi n) + aL}{4\pi^2 n^2}, n \in \mathbb{Z}. \tag{35}$$

Since $n \in \mathbb{Z}$, $\cos(2\pi n) = 1$ and $\sin(2\pi n) = 0$ and we finally obtain that:

$$E_n^{(1)} = \frac{aL}{2} + c, \tag{36}$$

So, finally, the first order approximation is the following:

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2} + \frac{aL}{2} + c \tag{37}$$

It is common in quantum mechanics to calculate second order corrections so according to [3], the second order corrections for the energy are given by the following equation:

$$E_n^{(2)} = \sum_{n \neq w} \frac{\left\langle \psi_w^{(0)} \left| V_1(x) \right| \psi_n^{(0)} \right\rangle}{E_n^{(0)} - E_w^{(0)}}. \tag{38}$$

So we have to calculate the following integral:

$$\left\langle \psi_w^{(0)} \left| V_1(x) \right| \psi_n^{(0)} \right\rangle = \int_0^L \frac{2(ax+c)\sin\left(\frac{\pi n x}{L}\right)\sin\left(\frac{\pi w x}{L}\right)}{L} \, dx. \tag{39}$$

After some calculations we finally arrive at the following result:

$$\left\langle \psi_w^{(0)} \left| V_1(x) \right| \psi_n^{(0)} \right\rangle = \frac{4aLnw\cos(\pi n)\cos(\pi w)}{\pi^2(n-w)^2(n+w)^2} \tag{40}$$

At this point it must be underlined that thanks to perturbation theory we are able to obtain similar results for the calculation of the wave function but this is not our primary goal in this letter. We aim to compare the results from different numerical approaches for the energy.

B. Taylor Expansion

In this section, we are going to use a different approach. By assuming that $L \sim \mathcal{O}(10^{-9})$ meters, we can calculate the Taylor expansion of (20) for $x << 1$ so we obtain the following equation:

$$\psi_t(x) = x\sqrt[3]{aA}\left(c_1 A_i'\left(\frac{A(c-E)}{(aA)^{2/3}}\right) + c_3 B_i'\left(\frac{A(c-E)}{(aA)^{2/3}}\right)\right) + c_1 A_i\left(\frac{A(c-E)}{(aA)^{2/3}}\right) + c_3 B_i\left(\frac{A(c-E)}{(aA)^{2/3}}\right). \tag{41}$$

From the boundary conditions, if we solve the equation $\psi(0) = 0$, we obtain that:

$$c_1 = -\frac{c_3 B_i\left(\frac{A(c-E)}{(aA)^{2/3}}\right)}{A_i\left(\frac{A(c-E)}{(aA)^{2/3}}\right)}, \tag{42}$$

and from the normalization of (41), we obtain that:

$$c_3 = \frac{\sqrt{3}}{\sqrt{\frac{L^3(aA)^{2/3}\left(A_i'\left(\frac{A(c-E)}{(aA)^{2/3}}\right)B_i\left(\frac{A(c-E)}{(aA)^{2/3}}\right) - A_i\left(\frac{A(c-E)}{(aA)^{2/3}}\right)B_i'\left(\frac{A(c-E)}{(aA)^{2/3}}\right)\right)^2}{A_i\left(\frac{A(c-E)}{(aA)^{2/3}}\right)^2}}}. \tag{43}$$

Bearing in mind the remaining equation obtained by the boundary conditions, $\psi(L) = 0$, we arrive at the following result:

$$E = c - \frac{a^{2/3}A^{(1)}(0)}{\sqrt[3]{A}}, \tag{44}$$

where $A^{(1)}(0)$ is the first zero of the Airy function, which is well known from the theory and Wolfram Mathematica© provides us the required value as $A^{(1)}(0) \approx 2.33811$.

C. Correlation between the approximation methods

In this section, our primary goal is to assert if results for energy provided in the previous sections can be considered as equal. From Taylor method, we obtained that:

$$E_t = \frac{2.3381a^{2/3}}{\sqrt[3]{A}} + c, \tag{45}$$

and from perturbation theory, we obtained that:

$$E_p = \frac{n^2\pi^2\hbar^2}{2mL^2} + \frac{aL}{2} + c + \sum_{n\neq w}\frac{1}{E_n^{(0)} - E_w^{(0)}}\left(\frac{4aLnw\cos(\pi n)\cos(\pi w)}{\pi^2(n-w)^2(n+w)^2}\right), \tag{46}$$

At this point, we have to define the following function:

$$D = E_p - E_t, \tag{47}$$

from which we able to calculate the difference between the obtained values from the different approaches. We are going to check our results if we assume that the particle is an electron, and according to [3], its mass is approximately $m_e \approx 0.511 \times 10^6$ eV/c^2. We have also to present the value of $\hbar$, which according to [3] is $\hbar \approx 6.58211 \times 10^{-16}$ eVs.

$$D = -1.7564 \times 10^{-12} a^{2/3} + \frac{aL}{2} + \frac{4.18388 \times 10^{-36} + 4.23916 \times 10^{-37} n^2}{L} \quad eV. \tag{48}$$

It is obvious that there are three unknown values in equation (48). At this point it has to be underlined that the constant c has been eliminated, making the calculations much more easier. If we recall that we have worked for $L \sim \mathcal{O}(10^{-9})$ meters, we have to check the possible values of D using contour plots, so we finally arrive at the following results:

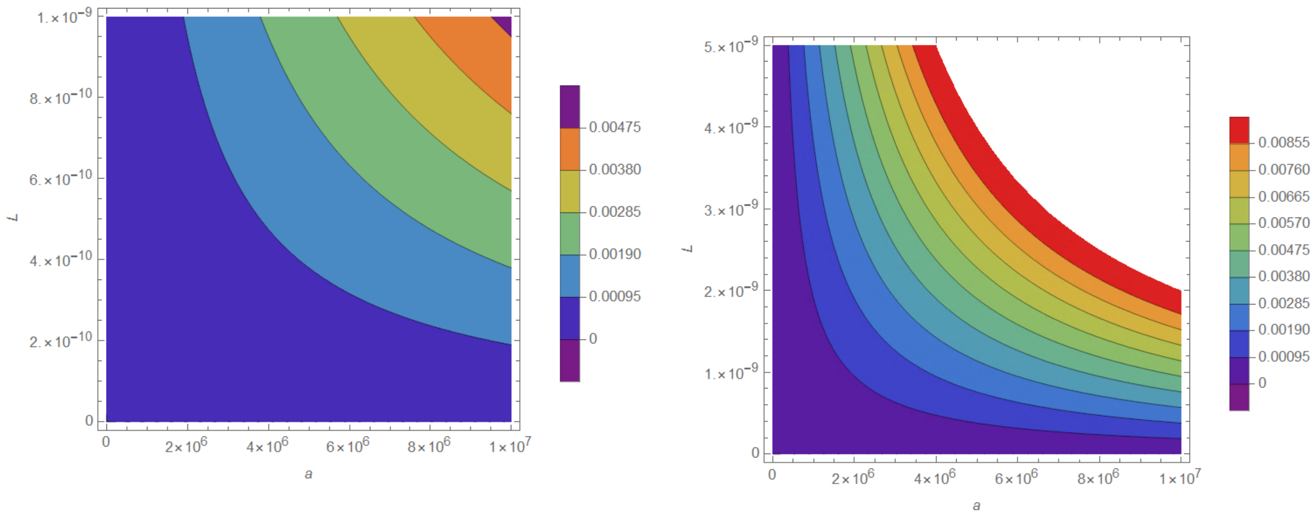


Figure 1: The accepted values of L and a if we demand $n = 1$ and $-0.01 \leq D \leq 0.01$, for $L \in [0, 10^{-9}]$ (left plot) and $L \in [0, 5 \times 10^{-9}]$ (right plot).

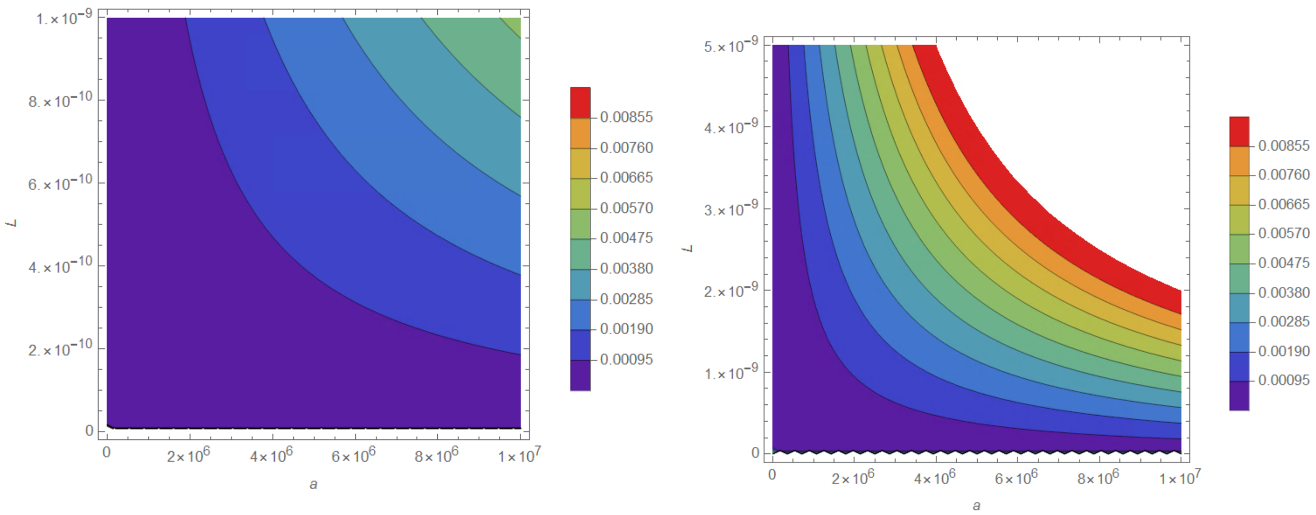


Figure 2: The accepted values of L and a if we demand $n = 10^{11}$ and $-0.01 \leq D \leq 0.01$, for $L \in [0, 10^{-9}]$ (left plot) and $L \in [0, 5 \times 10^{-9}]$ (right plot).

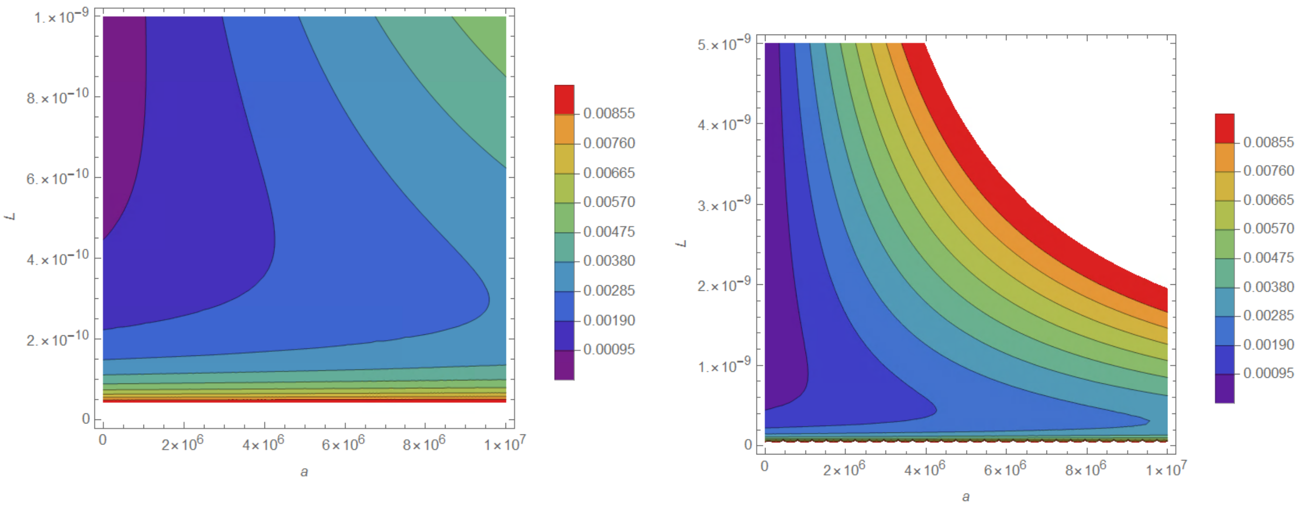


Figure 3: The accepted values of L and a if we demand $n = 10^{12}$ and $-0.01 \leq D \leq 0.01$, for $L \in [0, 10^{-9}]$ (left plot) and $L \in [0, 5 \times 10^{-9}]$ (right plot).

Thanks to figures 1, 2 and 3, we are able to assert that the two possible approaches may differentiate but the difference is not bigger than 1 % if $a \in [0, 10^7]$ and $L \in [0, 9 \times 10^{-9}]$. Last but not least, using different values of n thanks to Wolfram Mathematica© [8], we calculated that for $n \in [1, 1.44544 \times 10^{13}]$, the requirement $-0.01 \leq D \leq 0.01$ is still preserved.

III. POTENTIAL FORM $V(x) = \lambda x^2 + ax + c$, INSIDE THE INFINITE POTENTIAL WELL

We are going to proceed our analysis by introducing the following potential inside the infinite potential well:

$$V(x) = \lambda x^2 + ax + c \ , \ \ a > 0 \tag{49}$$

where

$$\mathcal{O}(a) = \mathcal{O}(\lambda) = \mathcal{O}(c). \tag{50}$$

and

$$a, c, \lambda << 1. \tag{51}$$

We chose the potential (49) because we can rely on the results obtained by the linear potential, and because it is a generalized case of the quantum harmonic oscillator, that is known for many physical applications. By recalling equation (6), after some simple calculations we obtain that:

$$\psi''(x) - \frac{2m}{\hbar^2}\left(\lambda x^2 + ax + c - E\right)\psi(x) = 0. \tag{52}$$

If we set $A = \frac{2m}{\hbar^2}$, we arrive at the following differential equation:

$$\psi''(x) - A\left(\lambda x^2 + ax + c - E\right)\psi(x) = 0. \tag{53}$$

In general the differential equation (53) is pretty difficult to be solved. A very simplified approach is to assume that $a^2 = 4c\lambda$, in this case $V(x) = \lambda x^2 + ax + c = (x + \frac{a}{2\lambda})^2$, so by setting $y = x + \frac{a}{2\lambda}$, we arrive at a well-known form, the quantum harmonic oscillator, which its solution is provided in almost every quantum mechanic book for educational purposes the author suggest the analysis provided by [2]. At this point, the reader should also recall that, the solution of the quantum harmonic oscillator is connected with the Hermite polynomials. The definition and the main properties of the aforementioned polynomials are provided by [5].

Since our goal is to solve the infinite potential well with the potential (49), we can use the perturbation theory approximation in order to obtain results. Initially, we will consider as perturbation the whole inserted potential provided by (49). Then, using the obtained result for the energy provided by (44) and the wave function given by (41), taking into account the equations (42) and (43), we will arrive to different result. Finally, we are going to examine the correlation between the different approaches demanding their difference to be smaller than 1%.

A. Considering $V(x) = \lambda x^2 + ax + c$ as perturbation

In the following subsection, we will consider $V(x) = \lambda x^2 + ax + c$ as perturbation, so recalling the equations (32) and (33), the following integral must be solved:

$$E_n^{(1)} = \int_0^L \frac{2\left(ax + c + \lambda^2 x^2\right)\sin\left(\frac{\pi n x}{L}\right)}{L} dx \Rightarrow \tag{54}$$

$$E_n^{(1)} = \frac{2\left(L\left(\pi^2 a(-1)^n n^2 + \lambda^2 L\left(\pi^2(-1)^n n^2 - 2(-1)^n + 2\right)\right) + \pi^2 c\left(\left(-1\right)^n - 1\right) n^2\right)}{\pi^3 n^3}, n \in \mathbb{Z} \Rightarrow \tag{55}$$

So, it is obvious that, we obtain different results if n is odd and if it is even. We will start by considering n as even and we will arrive at the following result:

$$E_{e,n}^{(1)} = -\frac{2L\left(a + \lambda^2 L\right)}{\pi n}, n \in \mathbb{Z}. \tag{56}$$

So, recalling, (33) we end up:

$$\widehat{E_{e,n}} = \frac{n^2\pi^2\hbar^2}{2mL^2} - \frac{2L\left(a + \lambda^2 L\right)}{\pi n}, n \in \mathbb{Z}. \tag{57}$$

The reader should not be confused because we symbolized the result again as $E_n^{(1)}$, it has nothing to do with the results from the II A. Now, we will consider n as odd, so we arrive at the following result:

$$E_{o,n}^{(1)} = \frac{2L\left(\pi^2 a n^2 + \lambda^2 L\left(\pi^2 n^2 - 4\right)\right) + 4\pi^2 c n^2}{\pi^3 n^3}, n \in \mathbb{Z}. \tag{58}$$

So recalling (33) we end up:

$$\widehat{E_{o,n}} = \frac{n^2\pi^2\hbar^2}{2mL^2} + \frac{2L\left(\pi^2 a n^2 + \lambda^2 L\left(\pi^2 n^2 - 4\right)\right) + 4\pi^2 c n^2}{\pi^3 n^3}, n \in \mathbb{Z}. \tag{59}$$

B. Considering $V(x) = \lambda x^2$ as perturbation

In this case, we are going to use the obtained result for the energy provided by (44) and the wave function given by (41), taking into account the equations (42) and (43). If we bear in mind the equations (32) and (33), the following integral must be solved:

$$\widehat{E^{(1)}} = \int_0^L \lambda x^2 \psi_t(x)^2 dx \Rightarrow \tag{60}$$

$$\widehat{E^{(1)}} = \frac{3\lambda L^2}{5}. \tag{61}$$

So, recalling, (33) we arrive at:

$$\widehat{E_p} = c - \frac{a^{2/3} A^{(1)}(0)}{\sqrt[3]{A}} + \frac{3\lambda L^2}{5} \tag{62}$$

C. Correlation between the approximation methods

Following our steps from II C, we will define again the following function:

$$G_e = \widehat{E_{e,n}} - \widehat{E_p}. \tag{63}$$

Bearing in mind the equations (57), (62), and the value of A obtained by our analysis in the previous section, we arrive at the following result:

$$G_e = \frac{1.75641a^{2/3}}{10^{12}} - \frac{0.63662L\left(a+\lambda^2 L\right)}{n} - c - 0.6\lambda L^2 + \frac{4.18388n^2}{10^{36}L^2}, n \in \mathbb{Z}, \tag{64}$$

since $\mathcal{O}(a) = \mathcal{O}(\lambda) = \mathcal{O}(c)$ we are able to simplify our result as:

$$G_e = -c + \frac{4.18388 \times 10^{-36} n^2}{L^2} - \frac{0.63662 \times La}{n} - 0.6L^2\lambda, n \in \mathbb{Z}, \tag{65}$$

and if we, finally, recall that $a, c, \lambda << 1$, we arrive at:

$$G_e = -c + \frac{4.18388 \times 10^{-36} n^2}{L^2} - \frac{0.63662 \times La}{n}, n \in \mathbb{Z}. \tag{66}$$

In order to achieve our goal, we need $\mathcal{O}(G_e) = \mathcal{O}(c)$. Since $n \in \mathbb{Z}$, as n grows bigger, the term $\frac{0.63662 \times La}{n}$ gets even smaller and since $\mathcal{O}(0.63662 \times La) < \mathcal{O}(c)$, so we can ignore this term as $n \to \infty$. At this point, we will turn our focus on the term $\frac{4.18388 \times 10^{-36} n^2}{L^2}$ where, again, we demand $\mathcal{O}(\frac{4.18388 \times 10^{-36} n^2}{L^2}) = \mathcal{O}(c)$, so we finally obtain that $\mathcal{O}(n) \leq 10^{16}$. This result proved that for slew of integers, the two approaches provide the same results. At this point, it must be denoted that, the results provided for energy in II B and III B are not quantized, even-though we demanded that our potential is inside the infinite well. This is the reason why, while examining the correlations in II C and III C, we extracted constrains for the values of n. At this point, we have to follow the same route by assuming that n is odd. We will define again the following function:

$$G_o = \widehat{E_{o,n}} - \widehat{E_p}. \tag{67}$$

Bearing in mind the equations (59), (62), and the value of A obtained by our analysis in the previous section, we arrive at the following result:

$$G_o = \frac{0.0322515\left(2L\left(9.8696an^2 + \lambda^2 L\left(9.8696n^2 - 4\right)\right) + 39.4784cn^2\right)}{n^3}, n \in \mathbb{Z} \Rightarrow \tag{68}$$

$$G_o = \frac{0.63662aL}{n} + \frac{1.27324c}{n} - \frac{0.258012\lambda^2 L^2}{n^3} + \frac{0.63662\lambda^2 L^2}{n}, n \in \mathbb{Z} \Rightarrow \tag{69}$$

since $\mathcal{O}(a) = \mathcal{O}(\lambda) = \mathcal{O}(c)$ and even if for $n = 1$ we are sure that $\mathcal{O}(G_o) < \mathcal{O}(c)$, so in this case for all $n \in \mathbb{Z}$, $\mathcal{O}(G_o) < \mathcal{O}(c)$.

IV. POTENTIAL FORM $V(x) = \frac{\hbar^2}{2m}x^\xi$, INSIDE THE INFINITE POTENTIAL WELL, SOLVED WITH FROBENIUS METHOD

In this section we are going to solve the S.E. using the Frobenius method. Firstly, let us introduce the following potential:

$$V(x) = \frac{\hbar^2}{2m}x^\xi \ , \ \xi \in \mathbb{Z} \ , \ x \geq 0 \tag{70}$$

Even if it seems rather strange hypothesizing (70), there are two advantages. Firstly, as ξ grows bigger, the behaviour of the potential is the following:

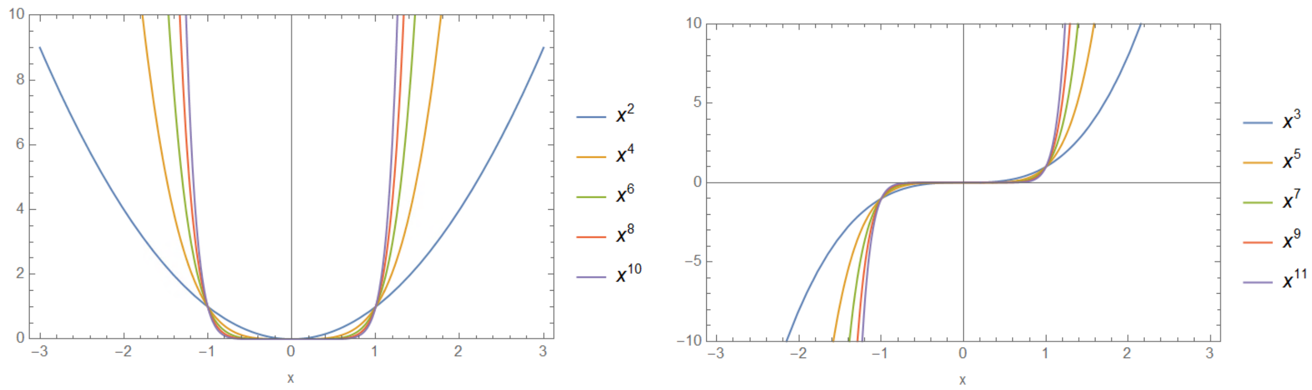


Figure 4: The plot of $f(x) = x^{\xi}$, for $\xi = 2, 4, 6, 8, 10$ (right plot) and $f(x) = x^{\xi}$, for $\xi = 3, 5, 7, 9, 11$ (left plot). $x \in [-3, 3]$

It must be denoted that in plots provided in figure 4, x can be also negative. We choose this kind of presentation to underline the different behaviour of (70) for $x < 0$ and the similar one for $x > 0$. The second reason for choosing (70) is that it is simplifies the S.E., so we finally arrive at:

$$\psi''(x) - \left(x^{\xi} + B\right)\psi(x) = 0, \tag{71}$$

where $B = -\frac{\hbar^2 E}{2m}$. Bearing in mind the Frobenius method provided in I A we arrive at:

$$\sum_{n=0}^{\infty} n(n-1)c_n x^{n-2} - (x^{\xi} + B)\sum_{n=0}^{\infty} c_n x^n = 0 \Rightarrow \tag{72}$$

$$\sum_{n=0}^{\infty} n(n-1)c_n x^{n-2} - \sum_{n=0}^{\infty} c_n x^{n+\xi} - \sum_{n=0}^{\infty} Bc_n x^n = 0. \tag{73}$$

At this point, we need to transform the series provided in equation (73), so not only the lowest limit of each term to be the same, but also the exponent of x to be the same, so after some simple calculations we arrive at:

$$S(x) + \sum_{n=0}^{\infty}(n+\xi+1)(n+\xi+2)c_{n+\xi+2}x^{n+\xi} - \sum_{n=0}^{\infty} c_n x^{n+\xi} - \sum_{n=0}^{\infty} Bc_{n+\xi}x^{n+\xi} = 0, \tag{74}$$

where $S(x)$ is the following:

$$S(x) = \sum_{n=-(\xi+2)}^{-1} (n+\xi+1)(n+\xi+2)c_{n+\xi+2}x^{n+\xi} - \sum_{n=-\xi}^{-1} Bc_{n+\xi}x^n. \tag{75}$$

At this point a reader familiar with the well-known solution of the quantum harmonic oscillator understands that we are following the same route to S.E. for the specific potential we introduced, if we set $\xi = 2$. If the reader is not familiar Stephen Gasiorowicz provides the solution in [2]. The main difficulty of our problem is that if we do not know ξ, finding the retroactive equations for the constants, required to solve S.E., becomes a rather complicated problem. So we are going to introduce a hypothesis to simplify our problem, that as we are going to prove, provides us a rather interesting result not only from a pure mathematical aspect, but also from a physical one. Our assumption is that if $x << 1$ and $\xi >> 1$, then:

$$S(x) + \sum_{n=0}^{\infty}(n+\xi+1)(n+\xi+2)c_{n+\xi+2}x^{n+\xi} - \sum_{n=0}^{\infty} c_n x^{n+\xi} - \sum_{n=0}^{\infty} Bc_{n+\xi}x^{n+\xi} \approx S(x). \tag{76}$$

This result leads us to an easier mathematical analysis to obtain a general result for the coefficients, so we end up for the following results:

$$c_{2k} = \frac{(-1)^k B^k}{(2k)!}c_0\ ,\ k \in \mathbb{Z}, \tag{77}$$

and

$$c_{2k+1} = \frac{(-1)^k B^k}{(2k+1)!} c_1 \ , \ k \in \mathbb{Z}. \tag{78}$$

Finally, we obtain that the general solution of (71) is the following:

$$\psi(x) \approx c_0 \sum_{k=0}^{[\xi/2]} \left(\frac{(-1)^k B^k}{(2k)!} \right) x^{2k} + c_1 \sum_{k=0}^{[\xi/2]} \left(\frac{(-1)^k B^k}{(2k+1)!} \right) x^{2k+1}. \tag{79}$$

An attentive reader can already understand, that if $\xi \to \infty$, then we are able to obtain the Maclaurin series of $\cos x$ and $\sin x$. To be more precise, according to [7] the Maclaurin series are the following:

$$\cos x = \sum_{k=0}^{\infty} (-1)^k \frac{x^{2k}}{(2k)!} \tag{80}$$

and

$$\sin x = \sum_{k=0}^{\infty} (-1)^k \frac{x^{2k+1}}{(2k+1)!} \tag{81}$$

So we can finally arrive at the following result, for $\xi \to \infty$:

$$\psi_\infty(x) = c_0 \cos\left(\sqrt{B}x\right) + c_1 \sin\left(\sqrt{B}x\right) \tag{82}$$

At this point we need to determine c_0 and c_1. Recalling the boundary conditions for the infinite potential well, we have that $\psi_\infty(0) = 0$, so $c_0 = 0$. At this point, just like for the classic problem, the equation $\psi_\infty(L) = 0$ requires that either $c_1 = 0$ or $\sin(\sqrt{B}L) = 0$. Obviously the second option has a physical meaning so we need to solve the equation $\sin(\sqrt{B}L) = 0 \Rightarrow \sqrt{B}L = n\pi$, where $n \in \mathbb{Z}$. Till this point we have not referred to the sign of, so for $E > 0 \Rightarrow B < 0$, after some simple calculations we arrive at:

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2}. \tag{83}$$

At this point we have to determine the remaining constant c_1, so from the normalization and taking into account the previous result we arrive at:

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}. \tag{84}$$

Obviously, thanks to our assumption we ended up with the well known solution for the infinite potential well. So the most important result we extracted, is that even if we insert a potential inside the infinite well, we can ignore it. At this point, we should ask ourselves a new question, how big should ξ be in order to ignore the inserted potential? If we rearrive at the equation (74) and try to solve the problem with the Frobenius method, sooner or later we are going to stumble on a hard and complicated mathematical problem. On the other hand we need to determine, whether we can or not ignore the inserted potential, so we will use perturbation theory, by assuming that the potential (70), inserts a perturbation, that it is small but not ignoreable. So following the well known route the correction of the first order is calculated as following:

$$E_n^{(1)} = \int_0^L \frac{2x^\xi \sin^2\left(\frac{\pi n x}{L}\right)}{AL} dx \Rightarrow \tag{85}$$

$$E_n^{(1)} = \frac{2L^\xi \left(-2\pi^2 n^2 \, {}_1F_2\left(\frac{\xi}{2} + \frac{3}{2}; \frac{3}{2}, \frac{\xi}{2} + \frac{5}{2}; -n^2\pi^2 \right) \right)}{A(\xi+1)(\xi+3)}, \xi, n \in \mathbb{Z}, \tag{86}$$

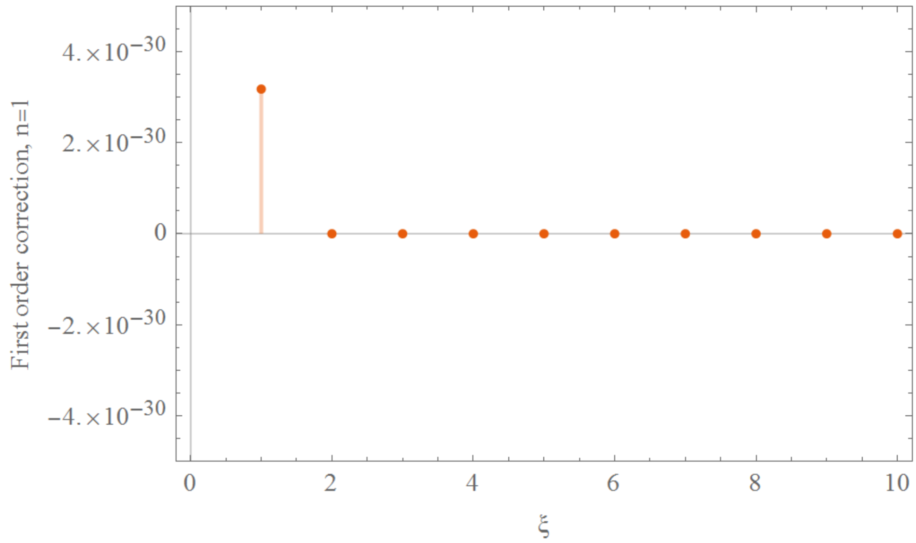
where ${}_pF_q(a; b; z)$ is the generalized hypergeometric function, for more details on the hypergeometric function, the reader should see [6]. So, we need to find how big should be ξ, to ignore $E_n^{(1)}$. It must be denoted that we will we work in S.I. and in order to obtain arithmetic results we will set $L = 10^{-9}m$, because this order of length, is the common in quantum mechanics. If our primary goal was to obtain a general constrain for ξ, the following inequality should be solved:

$$\frac{2L^{\xi}\left(-2\pi^2 n^2\,{}_1F_2\left(\frac{\xi}{2}+\frac{3}{2};\frac{3}{2},\frac{\xi}{2}+\frac{5}{2};-n^2\pi^2\right)\right)}{A(\xi+1)(\xi+3)} \leq \mathcal{O}(E_n \times 10^{-2}), \tag{87}$$

where E_n is the energy states of the unperturbed problem. As we can understand an analytical solution is hard to be obtained, if not impossible. So after some simple calculations we arrive at:

$$E_n^{(1)} = -\frac{2.50867 10^{9-\xi} n^2\,{}_1F_2\left(0.5\xi+1.5;1.5,0.5\xi+2.5;-9.8696n^2\right)}{10^{19}((\xi+1)(\xi+3))}, \tag{88}$$

at this point we could calculate the contour plot of the equation of (88), but even Wolfram Mathematica© [8] can not provide a contour plot, because the inserted values are incredibly small. So to be able to provide answer for our question we have to set specific values of n and the for each one of the find the discrete plot of (88). So we finally find the following plots:



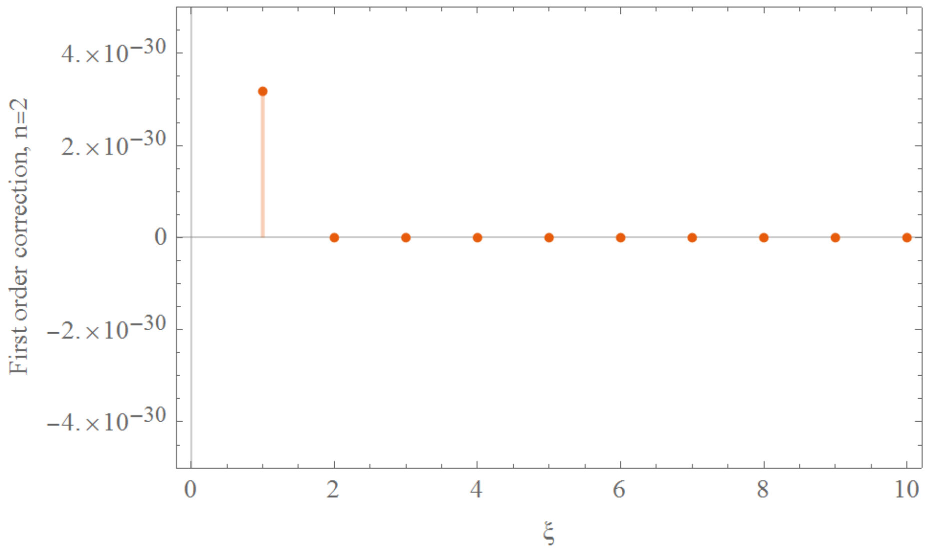


Figure 5: The contribution of the correction from perturbation theory for $n = 1$ and $n = 2$, for $\xi \in [1, 10], \xi \in \mathbb{Z}$

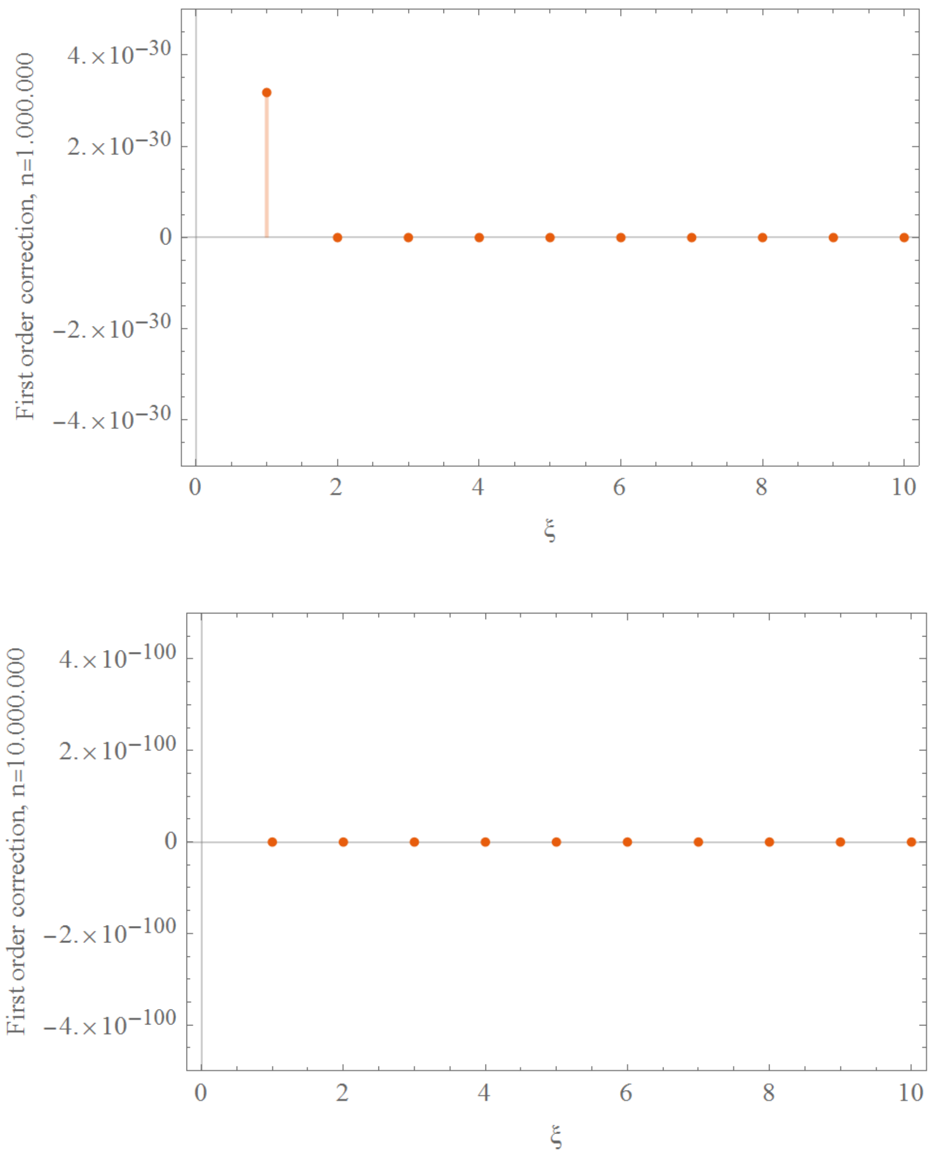


Figure 6: The contribution of the correction from perturbation theory for $n = 10^6$ and $n = 10^7$, for $\xi \in [1, 10], \xi \in \mathbb{Z}$

These results guarantee that for $\xi > 3$, our assumption is correct.

V. CONCLUSION

In this letter, we introduced the solution of the infinite well. Then, we inserted a linear potential, where we proved that it is not possible to obtain a direct solution.Thanks to perturbation theory and mathematical approximations, we obtained different results, that turned out to be close. Similar work have been done for the parabolic potential. Then, we proved that the difference between the two different approaches, for the different potentials, is smaller than 1 %, for a wide variety of the free parameters inserted in our problem. Last but not least, we introduced a monomial potential and we provided an approximate solution, using the Frobenius method and mathematical approximations. The aforementioned approximations led us to the well-known energy states of the infinite potential. So using perturbation theory we proved that out assumption could give acceptable results not just for $\xi \to \infty$. The reader could also check the Wolfram Mathematica© [8] notebooks provided in `https://github.com/reviskostis/Approximate-solutions-of-Schroedinger-equation-and-Frobenius-method`.

VI. ACKNOWLEDGEMENTS

In this letter the complicated calculations have been performed using Wolfram Mathematica© [8]. I would like also to thank Dr. Damianos Iosifidis for his comments on this paper and Dr. Vasilis K. Oikonomou for the tremendous help and the advises throughout my undergraduate years.

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