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SIMPLE LEARNING USING GOAL SEEK (MICROSOFT EXCEL) ABOUT ANHARMONIC OSCILLATOR POTENTIALS IN QUANTUM MECHANICS CLASS

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ABSTRACT

The completion of Schrödinger's anharmonic oscillator potentials equation in this Quantum Mechanics can be done with several methods such as using analysis method which is Perturbation Theory, Heun polynomials and Hamiltonians approach. It also can be done using numeric analysis method such as Runge-Kutta, Shooting Method, Numerov Method and so forth. However, those methods take a lot of time to solve the Schrödinger's equation on anharmonic oscillator potentials because it requires student's knowledge of the mathematic concept to solve the equation. Therefore, this paper will explain simple quantum mechanics learning particularly on the anharmonic oscillator lesson. As a result, students are expected to learn more in order to understand the quantum mechanics concept compared to understanding the equation of the completion methods concept. The method used is by using the basic Euler method with the help of Goal Seek data analysis on Microsoft Excel. From the result of the simulation using Goal Seek data analysis, E value is earned for each E_n energy level with the value variety γ=0 to 0.1 with the n quantum number from n=0 to n=20. In addition, this paper also gets the waves function graphic Ψ_n and probability $|\Psi_n|^2$ with the n quantum number from n=0 to n=3, as well as the waves function graphic equation Ψ_0 on n=0 with the value variety γ=0.05, 0.075, and 0.1. In addition, it also gets the waves function graphic equation Ψ_0 on n=0 with anharmonic oscillator potentials and simple harmonic oscillators. With this method, the students are expected to understand more about the concept of quantum mechanics particularly about anharmonic oscillator potentials.

Keywords: quantum mechanics, anharmonic oscillator potentials, euler method, goal seek

INTRODUCTION

Quantum mechanics is one of the courses that is relatively difficult for physics undergraduate students. This is caused by the difference of paradigm and classic mechanics which includes a mathematic knowledge for advanced level. One of the difficulties of quantum mechanics discussed in this paper is the anharmonic oscillator potentials concept that figures the atom's oscillation movement in a crystal around the balanced point. In order to get the figure of the quantum oscillation, it needs a solution of the Schrödinger's equation with spring potential V(x) of anharmonic oscillator. It is known that the solution of Schrödinger's equation for anharmonic oscillator potential is Hermits polynomial that is brought from the perturbation theory analysis, Heun polynomial, or even from the Halmiltonian approach. To get to that step, strong mathematic knowledge is usually needed about the differentials equation, line solution, and also the convergence features. This is what makes the quantum mechanics difficult for students in understanding the concept, especially for the anharmonic oscillator potentials.

In addition, there is another method that has been used to solve the Schrödinger's equation in anharmonic oscillator potentials which is using the numeric analysis method such as using Runge-Kutta method. This method can solve the Schrödinger's equation by using single arithmetical operation. However, this method is hard to understand for most of the students because they have to solve a few numeric equation functions. Another method that is often used is Numerov method. This method manipulates the Schrödinger's equation using Taylor's series and change the structure of the equation. This Numerov has a difficulty level that is similar to Runge-Kutta method (Qinghe, 2012 and Tang, 2014). Therefore, this paper will explain about another technique that is relatively easy, which is with the Euler numeric approach that is paired with Goal Seek analysis that is available on Microsoft Excel. Although the accuracy of Euler method is not really good compared to other better numeric methods such as Numerov method or Runge-Kutta, Euler method is way easier to learn and the result can show the Schrödinger's equation solution especially for anharmonic oscillator potentials. By using the Goal Seek data analysis we can get the energy E_n values that is quantized and from the Euler numeric scheme we also can get the wave function graphic Ψ_n. The energy level values E_n will next to be analyzed using polynomial regression on Microsoft Excel. The result can be compared to the results of other methods.

In this paper, there will be a comparison between the results of energy level E_n from the Goal Seek data analysis and a recent research that was conducted by Benjamin (2012) with quantum number n from n=0 to n=20 with the variety γ=0 to 0.1 and also wave function graphic Ψ_n and probability $|\Psi_n|^2$ with quantum number n=0 to n=3. In addition, there will be an explanation about the comparison of simulation result of wave function graphic Ψ_n on n=0 with variety γ=0.05,0.075, and 0.1 and comparison of simple harmonic oscillators graphic with anharmonic oscillators.

Anharmonic Oscillator Potentials

In classic mechanics (Sergei, 2006), anharmonic oscillation is a particular mechanics where the object is oscillating moving with the effect of out force, that causes the conservative force becomes:

$$\vec{F} = -m\omega^2\vec{x} - 4\alpha x^3 \tag{1}$$

where m is mass, ω is angle frequency that is $2\pi f$, and 4α is an out force constant that is very small that causes the oscillation move not in a sinusoid form that the oscillation will form an series expense that has different side of waves.

$$x(t) = x_0(t) + \alpha x_1(t) + \alpha^2 x_2(t) + \ldots, \tag{2}$$

where $x_0(t)$ is :

$$x_0(t) = A\cos\omega_0 t \tag{3}$$

For potential energy V(x) owned by an object that can be brought from the equation (1). That potential energy V(x) is:

$$V(x) = -\int_0^x \vec{F}.d\vec{x} = \frac{1}{2}m\omega^2x^2 + \alpha x^4 \tag{4}$$

As in a way of quantum mechanics (Benjamin, 2012 and Marshall, 2012), Schrödinger's equation for one particle that is oscillating anharmonicly in a one dimension form (viewed from x-axis) is:

$$\frac{d^2\Psi(x)}{dx^2} + \frac{2m}{\hbar^2}\left(V(x) - E\right)\Psi(x) = 0 \tag{5}$$

If equation (4) is substituted into equation (5), the equation becomes:

$$\frac{d^2\Psi(x)}{dx^2} + \frac{2m}{\hbar^2}\left(\left(\frac{1}{2}m\omega^2x^2 + \alpha x^4\right) - E\right)\Psi(x) = 0 \tag{6}$$

From equation (6) we can see that the solution of wave function Ψ(x) depends on potential energy in equation (4). If equation (6) is solved, then it is not only the wave function that we can get but also the stationer energy situation from the system or in other word the energy forms that is quantized. The solving equation is considered to be difficult because it has to be solved with mathematic equation for advanced level (Marselo, 1992). Therefore, it needs a dimensionless analysis which is by assuming $x=\beta z$, $\beta^2=\hbar/m\omega$, $\gamma=2\alpha\hbar/m^2\omega^2$, and $\varepsilon=2E/\hbar\omega$, which makes the equation (6) can be written as (Benjamin, 2012):

$$\frac{d^2\Psi}{dz^2} + \left(z^2 + \gamma z^4 - \varepsilon\right)\Psi = 0$$

$$\frac{d^2\Psi}{dz^2} = \left(z^2 + \gamma z^4 - \varepsilon\right)\Psi \tag{7}$$

Equation (7) is modeled using Euler method so it can be analyzed easily using Microsoft Excel. In regular Quantum Mechanics text books, to find the energy level E_n for each situation from equation (6) it needs an approach which is position normalization in a form of eigen function (Marshall, 2012). In this paper the energy value E will be counted using Goal Seek data analysis on Microsoft Excel for each quantum number n.

METHODS

Equation (7) can be assumed into two forms of analysis differentials from Euler method which is:

$$\Psi'(z)\begin{cases} \dfrac{d\Psi}{dz} = \Phi & (8) \\[2ex] \dfrac{d\Phi}{dz} = \left(z^2 + \gamma z^4 - \varepsilon\right)\Psi & (9) \end{cases}$$

This assumption can be modeled using a regular Euler method which is (Richard, 2006):

$$Y'(z) = \frac{Y(z+\Delta z) - Y(z)}{\Delta z}$$

$$Y(z+\Delta z) = Y(z) + Y'(z)\Delta z \tag{10}$$

where Y′(z) is a first differential from Y(z) function that can be written as Ψ′(z). In this case, Y(z) can be stated in Ψ(z) form and Φ(z). z is a used data interval. In this paper, z value is used from z= -5 to z=5. Δz is a distance between district points in z interval. The amount of district points N that is used in this paper is N=2000. By using Δz=(5-(5))/(N-1), Δz is 0,0050025. Because the value of Δz is very small, then it can be considered as $\Delta z = dz$. Now, equation (8) and (9) can be written in form of equation (10) which is:

$$\Psi(z + dz) = \Psi(z) + \Phi(z)dz \quad (11)$$

and

$$\Phi(z + \Delta z) = \Phi(z) + (z^2 + \gamma z^4 - \varepsilon)\Psi(z + dz)dz \quad (12)$$

Before starting to count using Microsoft Excel, the limit value $\Psi(z)$ in first point is found before which on z=-5, $\Psi(z)$ value is zero and $\Phi(z)$ value is $1\text{x}10^{-10}$. Then, in the next z value, it uses equation (11) for $\Psi(z+dz)$ and equation (12) for $\Phi(z+dz)$.

To find ε value on each quantum number n=0 to n=20 with variety γ=0 to 0.1, add a first variable value. That value will be counted using Goal Seek data analysis method on Microsoft Excel. Goal Seek data analysis method functions as to find the values of invers function or to find function's value from the first function. The limit's requirement of value ε will be solved by using Goal Seek data analysis is from $\Psi(z)$ on z=-5 to z=5 must equals zero. The value ε shown in Table 1 (for n=0 to n=3 with γ=0.05, 0.075, and 0.1). after that, with the same method, the value of probability $|\Psi_n|^2$ can also be found for each quantum number n by solving the integral function $|\Psi_n|^2$ dz=1. The probability graphic $|\Psi_n|^2$ wave function for each quantum number n can be seen on Figure 4.

RESULTS AND DISCUSSION

1. Energy Level E_n

From the result of the simulation using Goal Seek data analysis method, value ε on each quantum number n is gained. In Table 1, the comparison between the result of Goal Seek data analysis and the recent research conducted by Benjamin (2012) with the quantum number n from n=0 to n=3 for variety γ=0.05; 0.075 and 0.1. Beside that, on Table 1 there's also the result of energy level E_n which quantized using Goal Seek data analysis from n=0 to n=3 with γ=0.05, 0.075, and 0.1.

Table 1. Comparison Between the Result of Goal Seek Data Analysis and the Recent Research Conducted by Benjamin (2012)

Quantum number n	Gamma γ	Goal Seek Numerical	Numerical (Benjamin, 2012)	Energy Level E_n with Goal Seek
0	0.05	1.03473	1.03473	0.517364
	0.075	1.05206	1.05043	0.526029
	0.1	1.06365	1.06529	0.531828
1	0.05	3.16721	3.16723	1.583608
	0.075	3.23966	3.23967	1.619831
	0.1	3.30506	3.30687	1.65253
2	0.05	5.41723	5.41726	2.708618
	0.075	5.59028	5.59031	2.79514
	0.1	5.74591	5.74796	2.872957
3	0.05	7.77022	7.77027	3.885109
	0.075	8.07711	8.07718	4.038558
	0.1	8.35262	8.35268	4.176306

From Table 1 we can see that value ε the result of Goal Seek data analysis numeric calculation has a value that is similar with the result of numeric calculation that is done by Benjamin (2012). One of the values that is similar is on n=0 with γ=0.075, value ε that is found from numeric calculation of goal seek data analysis is 1.05206, while according to Benjamin (2012), numerically value ε can be found in the amount of 1.05043. The difference between these values is 0.00163. That difference is still relatively small. This is causes by the level of accuracy in doing the numeric data on Microsoft Excel is still low compared to other numeric software. Thoroughly, the difference of the values is 0.000345. However, the numeric calculation by using Goal Seek data analysis shows the solution of Schrödinger's equation for anharmonic oscillator potentials.

From Table 1, we can see that the calculation of quantized energy level E_n from n=0 to n=3 with γ=0.05, 0.075, and 0.1. The value of energy level E_n is earned by the analogy that has been explained above which is $\varepsilon = 2E/\hbar\omega$. From the analogy:

$$E_n = \frac{\varepsilon_n}{2}\hbar\omega \qquad (13)$$

Equation (13) describes that the quantized energy based on the level of quantum number *n* that has value by $\varepsilon_n/2$ times $\hbar\omega$. Below on Figure 1, one of the quantized energy level E_n graphic n=0 to n=3 with γ=0.1.

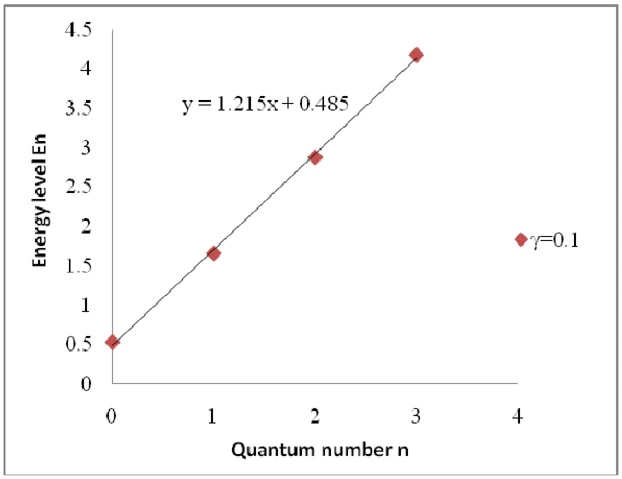


Figure 1. Comparison of quantum number *n* with quantized energy level E_n

Figure 1 is a result of linear regression analysis on Microsoft Excel with linear function y=1.215x+0.485. x variable is quantum number *n* while y is energy level E_n with γ=0.1 that is in Table 1. From graphic in Figure 1 we can see that the more the n value raises, the higher the energy level of E_n. This caused by the x variable factor which is the integer or in scientific point of view the x variable as the quantum number *n* which is n=0,1,2,3,..., Ideally the value of quantized energy level E_n in simple harmonic oscillators has a difference with anharmonic oscillator potentials (see Table 2).

Table 2. Comparison of Harmonic Oscillators Energy Level E_n with Anharmonics (γ=0.1)

Quantum number n	**E_n of Harmonics**	**E_n of Anharmonics (γ=0.1)**
0	0.49 $\hbar\omega$	0.53 $\hbar\omega$
1	1.49 $\hbar\omega$	1.65 $\hbar\omega$
2	2.49 $\hbar\omega$	2.87 $\hbar\omega$
3	3.49 $\hbar\omega$	4.17 $\hbar\omega$

In Table 2 seen the level energy E_n of simple harmonic oscillator comes with the equation:

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \quad n = 0,1,2,3... \qquad (14)$$

Whereas the anharmonics oscillator potentials does not follow the same equation. This is happened because of the disturbance of outern motion in the amount of γz^4 at the potential V(x).

In the research from Benjamin (2012), explained the function of value calculation series for each of quantum number *n* from n=0 to n=3 with the analysis of Pertubation theory (Table 3). In this paper also comes with the method of numeric calculation by using polynomial regression analysis provided in Microsoft Excel.

Table 3. The Comparison Equation of Pertubation Theory and Goal Seek Data Analysis

Nilai ε	**Pertubation Theory (Benjamin, 2012)**	**Goal Seek Analysis**
0	$1+0.75\gamma-1.3125\,\gamma^2+5.2031\,\gamma^3$	$1+0.824\,\gamma-3.749\,\gamma^2+22.90\,\gamma^3$
1	$3+3.75\gamma-10.3125\,\gamma^2+61.1718\,\gamma^3$	$3+3.708\,\gamma - 8.149\,\gamma^2+17.55\,\gamma^3$
2	$5+9.75\gamma-38.4375\,\gamma^2+313.7343\,\gamma^3$	$5+9.543\,\gamma- 27.30\,\gamma^2+66.58\,\gamma^3$
3	$7+18.75\gamma-98.4375\,\gamma^2+1044.1406\,\gamma^3$	$7+18.11\,\gamma- 62.47\,\gamma^2-166.0\,\gamma^3$

If the value γ added in the series function at the Table 3, we could get the slightly same result of value *ε* between the Pertubation theory and Goal Seek data analysis. For the example, value γ that is being used is γ=0.05 for n=0, then the value *ε* according to Pertubation theory is 1.0348, while based on the result of Goal Seek data analysis the value *ε* is 1.0346, with the difference value *ε* of 0.0002. As a whole, the average difference between the value *ε* of Perturbation theory with Goal Seek data analysis for each of value γ, are γ=0.05 is as 0.01, for γ=0.075 with the total amount 0.07 and 0.19.

Here is the graphic result of value γ from γ =0 to 0.1 with the quantum number *n* from n=0 to n=20.

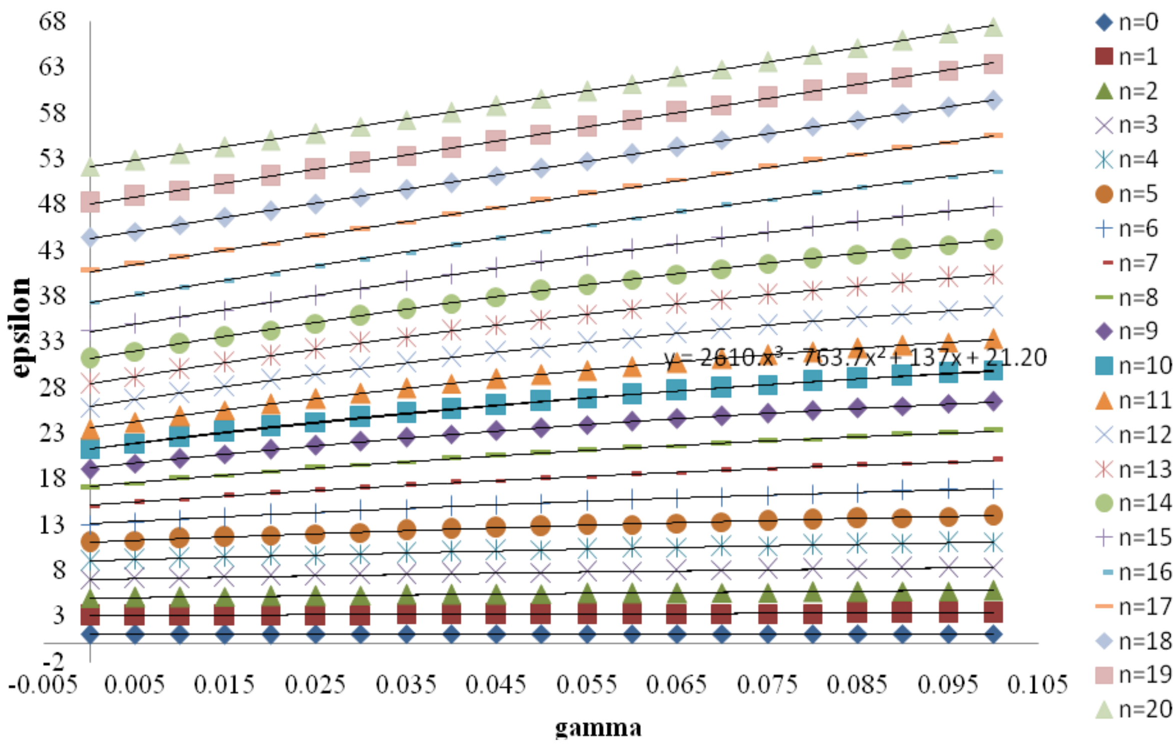
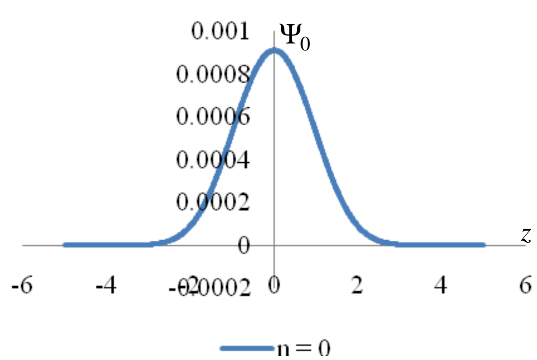


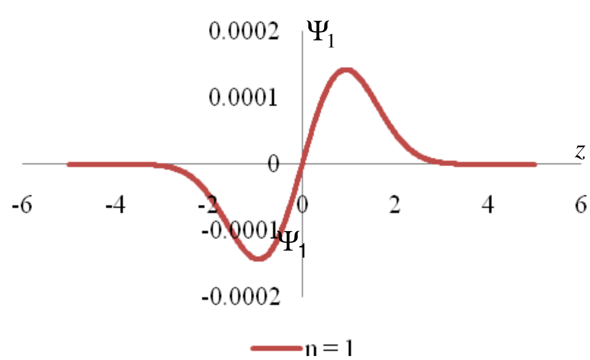
Figure 2. Spread of value ε with variation γ=0 to 0.1 at the quantum number *n* from n=0 to n=20

Figure 2 shows the graphic value ε as the result of polynomial analysis in the Microsoft Excel. For ε value of n=10 has been given the polynomial function that is $y = 2610x^3 - 763.7x^2 + 137x + 21.20$. In this case, where x is the value γ and y is the value ε. From that function we can get the value ε for n=10 (with γ =0.1) is 29.87. For n=15 polynomial function that we got is $y=-1779.x^3 - 40.45x^2 + 158.3x + 34.11$. Based on that function we get the value ε= 47.75 and for n=20 we get the polynomial function, which is $y=-1858.x^3 + 361.4x^2 + 135.5x + 52.18$. From this function achieved the value ε=67.48. Beside that, the graphic shown that if there are more n added, the value ε tend to raise to be linear. Seen in the n=0, value ε of γ=0 to 0.1 tend to be constant around the value ε 1.034, while n=20, the value ε inclined rise from 52.17 (at γ=0) to 67.48 (at γ=0.1). This is because the function of quartic potential z^4 function that is rising.

2. The Wave Function Ψ_n

The Figure 3 below shows the graphic of wave function Ψ_n from the calculation by using Goal Seek analysis. wave function Ψ_n that is presented come from the quantum number n=0 to n=3.





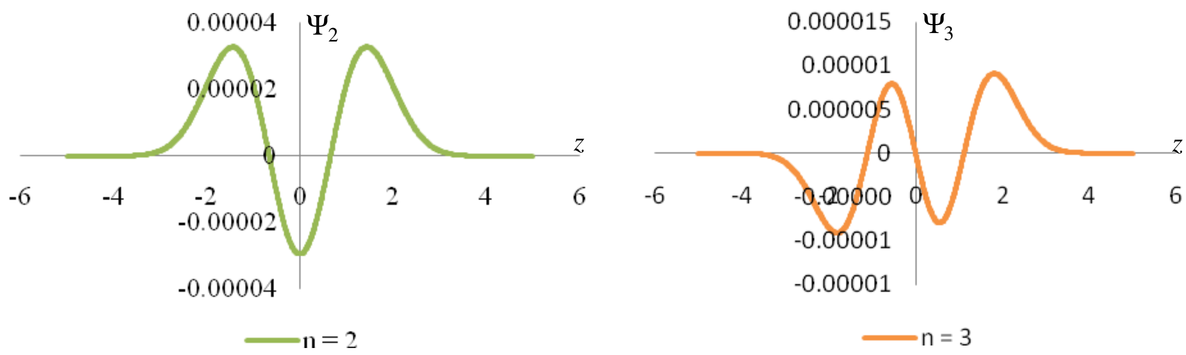


Figure 3. Graphic wave functions Ψ_n at the quantum number *n* from n=0 to n=3

Shown in the Figure 3 the variation shape of wave function at the quantum number n=0 to n=3. That variation of wave function has a strong connection with the energy level E_n. The variation of wave function caused by the potential V(x) that is different in each system lead to the differences in the level of energy. The wave function at the quantum number n=0 (basic state) that is located in the potential well V(x) can be interpreted that the wave function was being normalize. This means that the bigger the value z, the closer to zero the wave function Ψ_n is (Aditiya, 2009). Furthermore, the more quantum number *n* seen, the more wave produced. Scientifically speaking, we understand that the more quantum number *n*, the smaller the length of quantum wave λ produced.

3. Probability Functions $|\Psi_n|^2$

Probability $|\Psi_n|^2$ is the representation of the quadrate wave function Ψ that shows the possibility of having a particle in certain area or potential well in 1 dimension (Aditiya, 2009). The probability to find that particle described by a wave function in the dz interval around z point is $|\Psi_n|^2\, dz$ (Marcelo, 1992). Probability related with the probability requirement that the value must be a singular and normalized. Shown the probability graphic $|\Psi_n|^2$ in the anharmonic oscillator potentials with the quantum number *n* from n=0 to n=3.

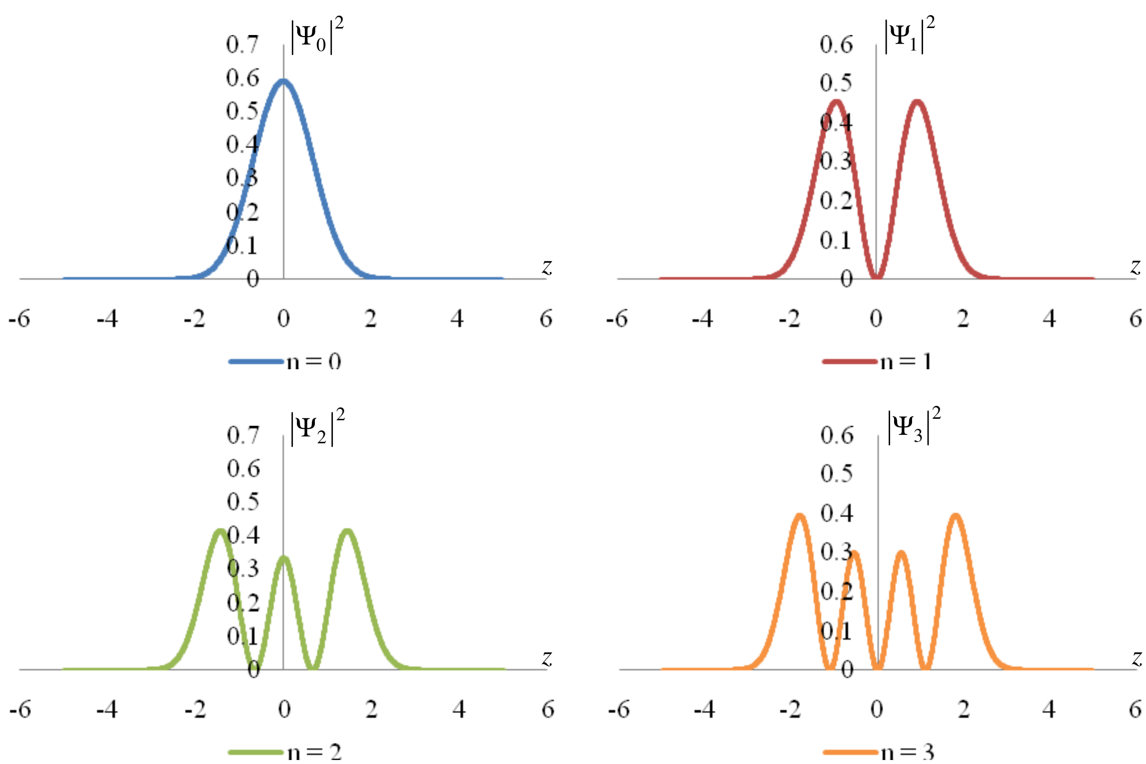
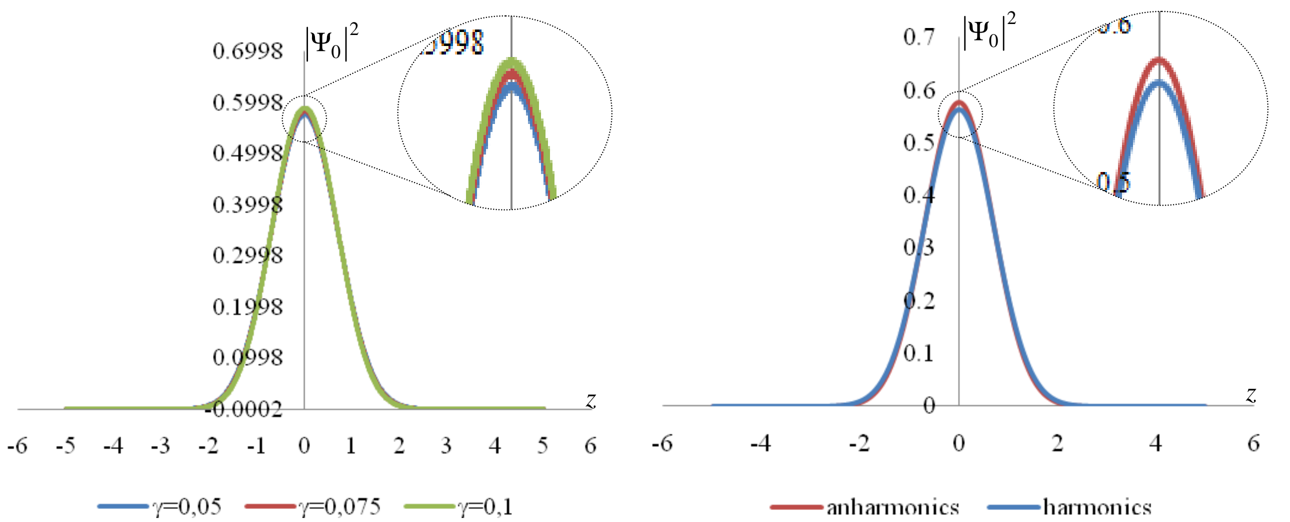


Figure 4. The probability $|\Psi_n|^2$ graphic with quantum number *n* from n=0 to n=3

Probability at n=0 shows the same shape with the quantum mechanics theory at the anharmonic oscillator potentials with the approach of Hermite polynomial. The shape of the graphic is more pointy compare to the wave function at n=0. In the graphic n=1 shows the probability value or the density of the biggest particle that can be found in the state of quantum number n=1. The more wave formed at n=3. Scientifically speaking, if there are many peak formed, then it will have a correspondence with the length wave of de Broglie. In the equation de Broglie, explained that the wave length reverse with the angle momentum. When the length of wave is smaller, the angle momentum will get bigger so the energy will be also much bigger. Shortly, the particle in this state (n=3) have the higher energy compare to the level energy below (n=0 to n=2), this conditioned the particle to move from one level of energy to the other level if there is an influence from the external motion. If the quantum number n added, then the particle energy that is going to be produced will get bigger and conditioned the particle to move from one level energy to the others.

Here is the graphic of comparison wave Ψ that has been normalized with the variation γ=0.05, 0.075, and 0.1 at the quantum number n=0 with the comparison graphic between simple harmonic oscillators with the anharmonic oscillator potentials.



(a) (b)

Figure 5. The comparison graphic of wave function Ψ_0 that has been normalized with the variation γ=0.05, 0.075, and 0.1 at n=0, (b) the comparison graphic between simple harmonic oscillators with anharmonic oscillator potentials at n=0.

In the Figure 5(a), shown the difference peak among the tree graphic at the state n=0, the blue graphic as the wave function with γ=0.05, the red graphic as the wave function with γ=0.075, and the green graphic as the wave function with γ=0.1. The figure shows that the more value γ added, the higher the peak of the wave function. In the Figure 5(b), is the graphic comparison between wave function between simple harmonic oscillators with anharmonic oscillator potentials. The blue graphic is the harmonic wave function while the red one is the anharmonic wave function. The amount of γ carried by itself is γ=0.05.

CONCLUSION

Euler numeric approach combine with Goal Seek data analysis provided in Microsoft excel able to show the solution of Schrödinger's equation. This method is one of the relatively easiest method for undergraduate student of physics program in dealing with the subject of quantum mechanics. Hopefully, there will be more student have a better understanding about the concept of quantum mechanics, especially in during the discussion of anharmonic oscillator potentials.

REFERENCES

Aditiya. 2009. *Pengkajian Osilator Harmonik Secara Kuantum dengan Simulasi Menggunakan Bahasa Pemograman Delphi 7.0*. Skripsi Universitas Sebelas Maret Surakarta.

Benjamin, T.F. 2012. Anharmonic Oscillator Potential: Exact and Pertubation Result. *Journal of Undergraduate Research in Physics*. 2012.

Marcelo A. & Edward J. Finn. 1992. *Dasar-dasar Fisika Universitas.* Edisi kedua. Penerbit Erlangga.

Marshall, L. B. 2012. *Modern Physics for Science and Engineering*, Tuskegee University, 401-403.

Qinghe, M., 2012. An Optimized Runge-Kutta Method for Numerical Solution of the Radial Schrödinger Equation. *Hindawi Publishing Corporation Mathematical Problems in Engineering,* Vol. 2012, 12 pages.

Richard B. & Gabriel C. 2006. *Persamaan Diferensial.* Edisi ketiga. Penerbit Erlangga, 121-123.

Roger, G., & Newton. 2001. *Quantum Physics-A text for Graduation Students*, New York, 82-85.

Sergei, W. 2006. *Pertubation Theory for Anharmonic Oscillations*. Lecture notes. 8 pages.

Tang, Dongjiao. 2014. Generalized Matrix Numerov Solution to the Schrödinger Equation. *National University of Singapore*, 25-28.