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Introducing Undergraduate Students to Nonlinear Dynamics through A Numerical Approach

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Abstract

This paper describes a numerical method that used to solve the nonlinear Schrödinger equation. The methods are an exponential time differencing method and a spectral method. The result indicates that at a certain parameter, fluctuation of wave function has contained chaotic dynamics. This case is expected to be used as an example for introducing numerical methods to undergraduate students on nonlinear dynamics. This introduction is deemed necessary, referring to the curriculum and syllabus used in several educational institutions in various countries that have included the topic of nonlinearity.

Keywords: nonlinear Schrödinger equation, exponential time differencing, spectral method, chaotic

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Introduction

There are several branches of physics that can be referred as the pillars of physics. Those pillars are classical mechanics, electromagnetism, optics, thermodynamics and statistical physics, quantum mechanics, and the theory of relativity. For undergraduate students whether in educational or non-educational physics, the subject must be mastered as a provision after they graduate and become physicists and physics teacher. Those pillars of physics have been included in the curriculum of each physics and physics education programme so that the objectives of the study programme which are to provide basic capabilities can be achieved. However, it is important to be remembered that physics will develop continuously, so that the pillars of physics can experience the transformation and addition.

One of the new branches of physics is linear dynamics which specifically chaos. In several countries, the topic of nonlinear dynamics has been included in the curriculum entitled Nonlinear Dynamics at North Carolina University [1], Nonlinear Physics: Modeling Chaos and Complexity at the University of California [2], Undergraduate Nonlinear Dynamics course at Cal Poly-San Luis Obispo [3], An Introduction to and Survey of Nonlinear Dynamics at Duke University [4], and Introduction to Nonlinear Dynamics at the Indian Institute of Technology [5]. Even, the topics specially had been discussed in the association of American physicists [6]. One of the reasons for the introduction of the topic into physics curricula is that this type of dynamic arises in many systems (both in nature and man made systems) and devices used in experiments and even in everyday life [7].

Based on the information above, it is time for nonlinear and chaotic topics to enter the curriculum in Indonesia. For this reason, one of the ideas will be presented in this article to introduce nonlinear and chaotic topics which are suitable for the situation of education and infrastructure in Indonesia through a computational numerical approach.

Methods

A mathematical model will be chosen is a nonlinear Schrödinger equation [8] as follows

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi + \alpha|\psi|^2\psi \quad (1)$$

where $\hbar$, m, V, ψ, and α are reduced Planck constant, mass, potential energy, wave functions, and interaction constant, respectively. The reason why choosing this equation is undergraduate students already know the Schrödinger equation from the quantum physics course. In other words, they already have a sufficient base of understanding and can follow the development in a nonlinear case. The difference in Equation (1) with the linear Schrödinger equation is at the last term, which is a nonlinear term.

The numerical approach will be discussed are an integration and a pseudo spectral method. For the integration method, Exponential Time Differencing (ETD) method is chosen to solve the time-dependent derivative equation. First, we assume there is a derivative equation with time as follows

$$\begin{aligned}\frac{\mathrm{d}u(t)}{\mathrm{d}t} &= cu(t) + F(u,t)\\ \frac{\mathrm{d}u(t)}{\mathrm{d}t} - cu(t) &= F(u,t) \quad (2)\end{aligned}$$

where c is constant and u is time-dependent function of t. Integration factor for Equation (2) is obtained by

$$\begin{aligned}\frac{\mathrm{d}v(t)}{\mathrm{d}t} &= -c\\ e^{v(t)} &= e^{-ct} \quad (3)\end{aligned}$$

and

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\left[e^{-ct}u(t)\right] &= -ce^{-ct}u(t) + e^{-ct}\frac{\mathrm{d}u(t)}{\mathrm{d}t}\\ &= e^{-ct}\left[-cu(t) + \frac{\mathrm{d}u(t)}{\mathrm{d}t}\right]\\ &= e^{-ct}F(u,t). \quad (4)\end{aligned}$$

Now, we integrate Equation (4) with boundary $t = t_n$ to $t = t_{n+1}$ and we define time steps as $h = t_{n+1} - t_n$. So Equation (4) can be written as integral form as follows

$$\begin{aligned}\int_{t_n}^{t_{n+1}} \mathrm{d}\left(e^{-ct}u(t)\right) &= \int_{t_n}^{t_{n+1}} e^{-ct}F(u,t)\,\mathrm{d}t \Leftrightarrow\\ \int_0^h \mathrm{d}\left(e^{-ct}u(t)\right) &= \int_0^h e^{-ct}F(u,t)\,\mathrm{d}t \quad (5)\end{aligned}$$

and then Equation (5) can be gradually solved as

$$\begin{aligned}\left[e^{-ct}u(t)\right]_0^h &= \int_0^h e^{-ct}F(u,t)\,\mathrm{d}t\\ e^{-ch}u(h) - \ldots & \\ e^{-c0}u(0) &= \int_0^h e^{-ct}F(u,t)\,\mathrm{d}t\\ \left(\frac{u(h)}{e^{ch}}\right) &= u(0) + \int_0^h e^{-ct}F(u,t)\,\mathrm{d}t\\ u(h) &= e^{ch}u(0) + e^{ch}\int_0^h e^{-ct}F(u,t)\,\mathrm{d}t\\ u(t_{n+1}) &= e^{ch}u(t_n) + \ldots\\ & e^{ch}\int_0^h e^{-ct}F(u_{t_n+\tau}, t_n+\tau)\,\mathrm{d}\tau\,. \quad (6)\end{aligned}$$

If $F(u_{t_n+\tau}, t_n+\tau)$ is constant and an approach can be made namely $u(t_n) = u_n$ and $F(u_n, t_n) = F_n$. We can simplify Equation (6) into

$$u_{n+1} = u_n e^{ch} + e^{ch}\int_0^h e^{-c\tau}F_n\,\mathrm{d}\tau \quad (7)$$

then

$$\begin{aligned}u_{n+1} &= u_n e^{ch} + e^{ch}F_n\left[-\frac{e^{-c\tau}}{c}\right]_0^h\\ &= u_n e^{ch} + \left(-\frac{e^{ch}F_n e^{-ch}}{c} + \frac{e^{ch}F_n e^{-c0}}{c}\right)\\ &= u_n e^{ch} + F_n\frac{(e^{ch}-1)}{c}. \quad (8)\end{aligned}$$

Equation (8) is first order of the Exponential Time Differencing method (ETD1) which has cutting error $\frac{h^2\dot{F}}{2}$.

Using the same method, the second ETD (ETD2) which has recursive expression can be obtained as follows [9–11]

$$\begin{aligned}u_{n+1} &= u_n e^{ch} + F_n\frac{\left((1+hc)e^{ch} - 1 - 2hc\right)}{hc^2} + \ldots\\ & F_{n-1}\frac{\left(-e^{ch} + 1 + hc\right)}{hc^2}. \quad (9)\end{aligned}$$

The ETD method (Equation (9)) is then combined with the discrete spectral method which has an expression

$$\psi(x) = \sum_{n=1}^{N}\psi_n e^{iK_n x} \quad (10)$$

where $K_n = \frac{2n\pi}{L}$ and ψ_n are Fourier coefficient. In general, the ETD2 method will be used to solve the time problem while the spectral method is applied to x as a function of position.

Results and Discussion

By applying the ETD2 and the spectral method, we can obtain a result of the nonlinear Schrödinger equation with a bistable potential as shown in Figure 1.

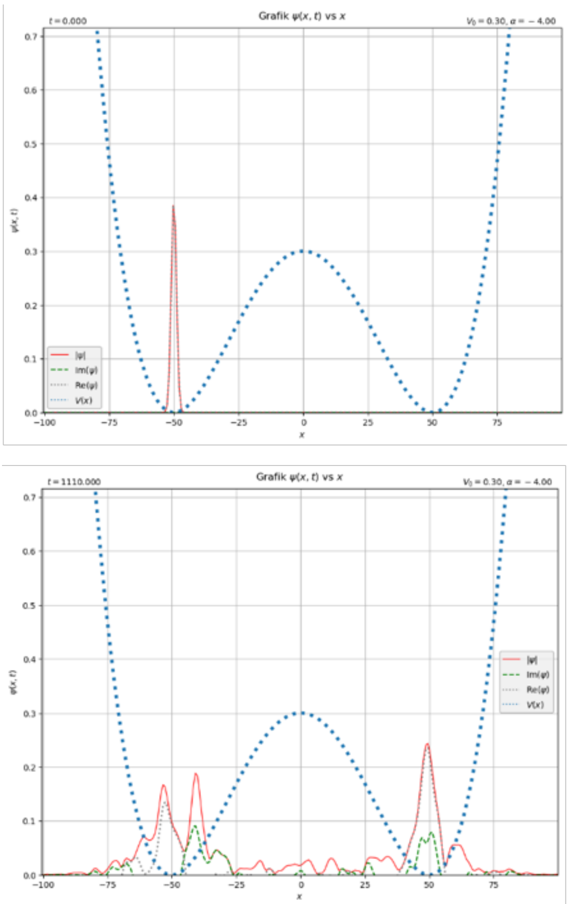

Figure 1: Snapshot of solution of Equation (1) with ETD2 and spectral method with interaction parameters $\alpha = -4$. The top panel is the initial condition where the wave function is on the stable side (left), while the lower panel shows a result at simulation with $t = 1110$ units of time.

Figure 1 shows that using proposed numerical approach, the simulation of Equation (1) which is a nonlinear differential equation can be done. For undergraduate students, those methods namely the series approach, integration, and Fourier transformation are actually taught to them. To be able to explain more quantitatively about dynamics, a statistical analysis of auto-correlation can be carried out by following equation

$$Q(x,\tau) = \left\langle \Delta\psi(x,t+\tau)\Delta\psi(x,t) \right\rangle_t \left\langle \Delta\psi(x,t)^2 \right\rangle^{-1} \quad (11)$$

where $\Delta\psi$ indicating the difference between ψ with a mean for all time and τ is the waiting time taken in the time step. Using Equation (11), we can obtain auto-correlation on some values of α as shown in Figure 2.

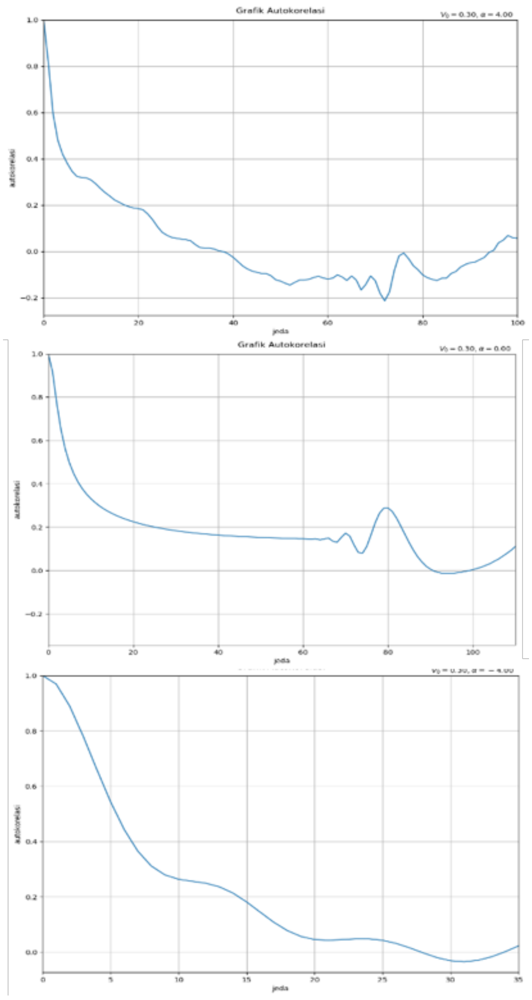

Figure 2: Auto-correlation of fluctuations ψ at $\alpha = 4$ (top), 0 (middle), and -4 (bottom), respectively.

Figure 2 shows that at $\alpha = 0$ decay of auto-correlation values occurs more slowly because the nonlinear term does not affect fluctuations in the solution of Equation (1). Whereas at $\alpha = -4$ and $\alpha = 4$, there is a rapid decay of auto-correlation values, in other words the nonlinear term plays a role and causes fluctuations that occur in the solution of Equation (1) become dominant.

In addition to auto-correlation, it can also be shown that there is an influence of the nonlinear term using the power spectrum of the solution fluctuations in Equation (1) which evolves with time as shown in Figure 3.

Figure 3 shows that at $\alpha = 4$ there are many peaks which indicate a number of frequencies that involved in wave function fluctuations. These characteristics also occurs at $\alpha = 0$, even though the position of the peaks increases compared to $\alpha = 4$. Both of these power spectra, there is no visible band as a background in the power spectrum, whereas at

$\alpha = -4$ bands as the background it is very visible. In addition, at $\alpha = -4$ there is still a dominant peak. The existence of a background band and dominant peak in the power spectrum is one indication that fluctuations in time-dependent wave function lead to chaotic dynamics.

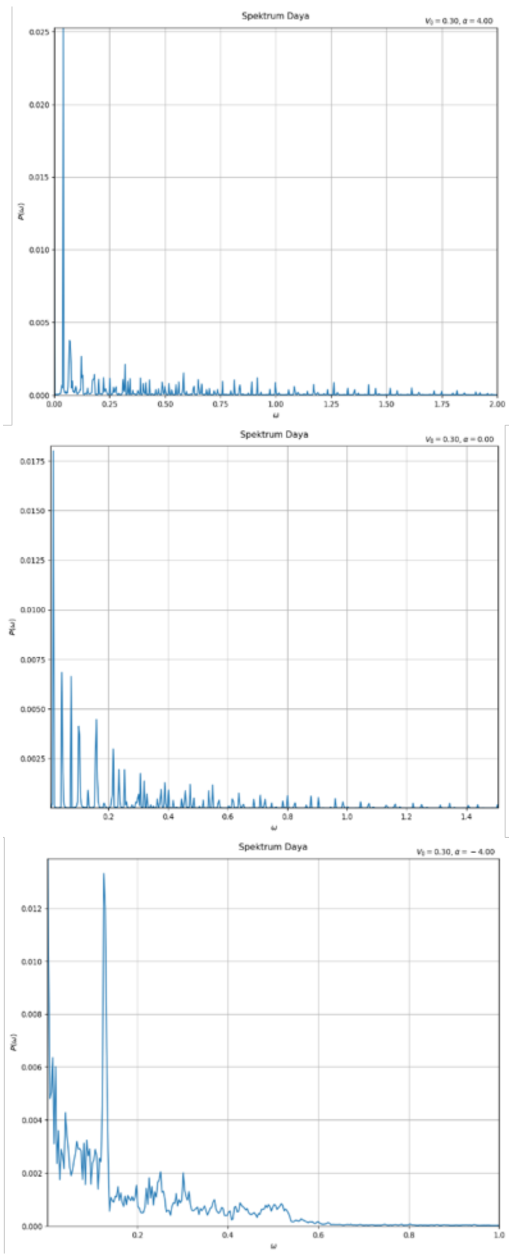

Figure 3: The power spectrum of fluctuations ψ at $\alpha = 4$ (above), 0 (middle), and -4 (bottom), respectively.

Conclusion

This paper has shown a computational method which can be used to solve the nonlinear Schrödinger equation. With the chosen method, it will obtain a numerical solution and will analyse the auto-correlation and power spectrum of obtained solution. The analysis shows that there is a complex dynamics and tend to be chaotic. This is one of the ideas for introducing linear dynamics to undergraduate students through the completion of the nonlinear Schrödinger equation although the proposed analysis only shows indication of chaotic dynamics. In other words, it is also necessary to introduce dynamic analysis such as Lyapunov's exponent. This analysis quantitatively will show that dynamics in the wave function as a solution of the nonlinear Schrödinger equation truly has had chaotic properties. Once again, the emphasis on this article is to introduce such dynamics to students.

Acknowledgments

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