

Dynamics of Two-Soliton Molecule with Impurities

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ABSTRACT

A soliton is the result of a delicate balance between dispersion-induced pulse self-broadening and nonlinearity-induced pulse self-narrowing, which brings in a constant propagation of the wave form and velocity. Additionally, soliton molecules are stable bound states that develop from two anti-phase bright solitons in a dipolar Bose-Einstein condensate, which represents another significant advance in the field. The behaviour of the two-soliton molecule of the nonlinear Schrödinger equation (NLSE) in the context of delta potential has been studied in this paper. Interaction of the solitons with the external potential will affect not only the speed, as classical particles do, but also the soliton's properties and its physical locations. This work seeks to resolve the non-integrable perturbed NLSE of the two-soliton molecule analytically using the variational approximation method (VAM). VAM gives dynamical equations for the parameters of the soliton in the form of ordinary differential equations, and it only creates approximation results. The accuracy of the results is checked numerically by direct numerical simulation. The split-step approach and Fast Fourier Transform are two coding techniques used in the direct numerical simulation method to assist in issue solving. The results indicated that, the two-soliton molecule may be reflected, transmitted through, or trapped within the external potential depending on the different potential strength.

Keywords: soliton, nonlinear Schrödinger equation, two-soliton molecule, variational analysis, Bose-Einstein condensate

INTRODUCTION

Initially observed in the domain of water waves, John Scott Russell made the first discovery of this phenomenon in August 1834 and after forth it is called as solitons or solitary waves. The concept of soliton has been established using a solution called Korteweg-de Vries (KdV) equation (Wadati, 2001). There are a few terms in this equation to characterize the nonlinear and dispersion effects. Particularly, it results in waveform steepening for nonlinear effects and waveform spreading for dispersion effects. These two effects are competing with each other and the fine balance between those effects leads to the existence of the stationary waveform or solitary wave.

According to Cattani and Bassalo (2013), the word “soliton” can be generally defined as a unique solitary wave such that its propagation is governed by a nonlinear equation and it possesses a spatial configuration where the nonlinearity of the medium is precisely counterbalanced by the dispersion or diffraction effects. Therefore, it is true that soliton is a wave but it can also move exactly like how a particle does. There are different kinds of solitons exist to solve different nonlinear equations, such as sine-Gordon equation and Nonlinear Schrödinger equation (NLSE) which is used in this study, apart from KdV equation itself. NLSE is described as having similar types with the propagation of optical pulses in both the anomalous dispersion regime (negative group velocity), and the normal dispersion regime (positive group velocity), as stated by Panoiu et al. (2000).

The scattering of matter wave solitons on localised potentials has been studied and received considerable attention for the past few years (Garnier and Abdullaev, 2006; Aklan and Umarov, 2015, 2017; Din et. al, 2020; Hansen et. al, 2021). While the study of two-soliton molecules (Al Khawaja, 2010; Umarov et. al 2016) is also widely debated for its different approaches analysis. The interaction force between multiple solitons was first studied by Karpman and Solov'ev using perturbation analysis, Hirota in 1972, who used the exact two solitons solution of the sine-Gordon equation, and Anderson and Lisak (1986) who employed a variational approach to incoherent two-soliton interaction.

The two-soliton molecules are two anti-phase bright solitons in a dipolar Bose-Einstein condensate (BEC) that can form stable bound states. The work will concentrate on the dynamics and scattering of a two-soliton molecule of a strong nonlocal NLSE by an external potential using analytically tractable Delta potential barriers and wells in spatial dimension. The discussion on the numerical simulations in terms of soliton molecules scattering by weak and strong potentials will be covered in the next section. The potential's strength and velocity of the collision will give substantial impact to the result of the soliton's scattering.

MAIN EQUATION

This study will use the Gross-Pitaevskii equation (GPE), which in general is the nonlinear Schrödinger equation (NLSE) as the main equation. This particular equation is convenient to use in the research of solitons. Based on Debnath (2005), the NLSE does not allow for a soliton solution representing a steady wave propagating with a constant velocity, which is different from the KdV equation. Moreover, an exponential function is represented for the plane wave part, and the amplitude of the sech profile propagates with different velocities. As a result, a solution known as an envelope soliton emerges, exhibiting particle-like behaviour. This phenomenon was numerically demonstrated by Yajima and Outi (1971) while, Zakharov and Shabat (1972) proved it analytically using the inverse scattering method. They discovered that this method gives an exact solution to the initial-value problem for the NLSE. In the process of addressing this problem, the concept of Lagrangian stability is introduced and the solution is $\psi(x, t)$ if constant K that is independent of t is exist, but possibly dependent on the initial data.

The governing equation NLSE includes its generalized form and external potential is used throughout the work. It is called perturbed NLSE as perturbation exists with the additional term of the external potential. Previous researchers have shown that by using the asymptotic perturbation technique, the pulse propagation can be described by the perturbed NLSE as used in this study (Mihalache et al., 1993). The main equation can be modelled in the following form,

$$i \frac{\partial \psi}{\partial t} + \frac{1}{2} \frac{\partial^2 \psi}{\partial x^2} - V(x)\psi + q|\psi|^2 \psi + g\psi \int_{-\infty}^{+\infty} R(|x-z|)|\psi(z, t)|^2 dz = 0, \quad (1)$$

where $\psi(x, t)$ denotes the mean-field wave function of the condensate, $V(x)$ indicates the presence of the external potential, q and g are the nonlinearity coefficients account for the condensate's short-range contact and long-range dipole-dipole interactions between atoms, respectively (Umarov et al., 2016). As the external potential added is not integrable, so the NLSE cannot be solved analytically. It is known that Inverse Scattering Transform (IST) can be used to solve integrable partial differential equation (PDE) such as NLSE but not for this perturbed NLSE. Therefore, variational approximation method is used to find the approximate solutions for this study and checked its accuracy by using the direct numerical simulation method. This method will be discussed in the next section.

The normalization condition of the wave function to the number of atoms within the condensate is written as

$$N = \int_{-\infty}^{+\infty} |\psi|^2 dx, \quad (2)$$

and Eq. (2) is known as the norm of the system. The norm is regarded as a conserved quantity of Eq. (1) where $dN/dt = 0$ for every trajectory. Next, supposed that the response function $R(x-z)$ is characterized by

$$R(x-z) = \frac{1}{\sqrt{2\pi}w} \exp\left(-\frac{(x-z)^2}{2w^2}\right), \quad (3)$$

where w is the width of the potential, and is normalized, $\int_{-\infty}^{\infty} R(x-z)dx = 1$. The response function defines the medium's level of nonlocality. Particularly, it demonstrates how closely the characteristics of the medium depend on those of its surrounding regions at a specific position. According to Umarov et al. (2016), the response function for contact interactions is the same the Dirac delta function where the particles can only affect one another when they are at a similar spatial location. Meanwhile, the response function for the long-range dipole-dipole interactions is considered to take the form as in Eq. (3).

We examined the interaction of a two-soliton molecule with an external potential that has the form of a Delta function given by

$$V(x) = -U_0 \delta(x), \quad (4)$$

and U_0 corresponds to the strength of the potential. In general, the shape of the potential can be classified based on the value of potential strength. For the positive value of U_0 , the potential has the shape of a potential wall whereas for the negative value of U_0 , the potential has the shape of a potential well.

VARIATIONAL ANALYSIS: VARIATIONAL APPROXIMATION METHOD

Variational approximation method (VAM) was first introduced by Anderson in 1983. In previous years, numerical investigations are often used to solve the convoluted form of the exact solution for the nonlinear Schrödinger equation (NLSE) and it becomes a complementary tool to understand the properties of the NLSE (Satsuma & Yajima, 1974). Other than the numerical method, the approximate analytical results are also needed to be obtained as it is useful in further understanding the physical phenomena between dispersion and nonlinear effects in optical fibers related to the propagation of the pulse. To get the approximate solutions, nevertheless, some of the more specific information of the solutions are need to be sacrificed.

Anderson used a variational approach to illustrate the main characteristics of the soliton dynamics governed by the NLSE on the basis of trial functions. Prior research on the nonlinear self-focusing of laser beams used this method and achieved successful agreement with the numerical results (Anderson & Bonnedal, 1979). There are some main advantages of variational approach that have been mentioned by Anderson such as this approach provides a clear analytical expression for the most significant parameters, including pulse compression or decompression factor, the maximum amplitude and the induced frequency chirp, which describes the propagation of the solitons, even though it is approximate.

Using the same approach, we develop the method for our particular case. To begin, we derive the Lagrangian density of Eq. (1) as follows,

$$L = \frac{i}{2}(\psi\psi_t^* - \psi^*\psi_t) + \frac{1}{2}|\psi_x|^2 + V(x)|\psi|^2 - \frac{q}{2}|\psi|^4 - \frac{g}{2}|\psi(x,t)|^2 \int_{-\infty}^{+\infty} R(|x-z|)|\psi(z,t)|^2 dz. \quad (5)$$

By utilizing the Euler-Lagrange equation below,

$$\frac{d}{dt} \frac{\partial L}{\partial \left(\frac{\partial \psi^*}{\partial t} \right)} + \frac{d}{dx} \frac{\partial L}{\partial \left(\frac{\partial \psi^*}{\partial x} \right)} - \frac{\partial L}{\partial \psi^*} = 0, \quad (6)$$

it can be easily verified that the above Lagrangian of Eq. (5) can generate the system in Eq. (1) corresponding to the following variational principle,

$$\delta \iint L \left(\psi, \psi^*, \frac{\partial \psi}{\partial x}, \frac{\partial \psi^*}{\partial x}, \frac{\partial \psi}{\partial t}, \frac{\partial \psi^*}{\partial t} \right) dx dt = 0. \quad (7)$$

Next, choosing a suitable trial function is the most critical step in developing the VA method as it will determine the success of the method. Commonly, many of the literature used Gaussian profile as the trial function since the variational equations obtained will particularly reproduce the exact solution of Eq. (1) (Anderson, 1983). The chosen trial function for our case is the first Gauss-Hermite function as being applied by Umarov et al. (2016) which has the form as below,

$$\psi(x,t) = A(x-\xi) \exp \left(-\frac{(x-\xi)^2}{2a^2} + ib(x-\xi)^2 + iv(x-\xi) + i\varphi \right), \quad (8)$$

where $A(t)$, $a(t)$, $\xi(t)$, $b(t)$, $v(t)$ and $\varphi(t)$ are the time-dependent amplitude, width, center-of-mass position, chirp, velocity and phase of the soliton molecule, respectively. The velocity v is specified as a derivative of the center-of-mass position of the soliton molecule with respect to time t such that $v = \xi_t$. The norm is calculated to be $N = A^2 a^3 \sqrt{\pi}/2$ and it is proportional to the number of atoms in the condensate.

The Lagrangian density in Eq. (5) is then re-expressed by using the response function in Eq. (3) and the ansatz in Eq. (8). Consequently, we evaluate the effective Lagrangian by solving the spatial integration of each term in the Lagrangian density where $L = \int_{-\infty}^{+\infty} L_G dx$ and L_G represents the results obtained from substituting the Gauss-Hermite ansatz into the Lagrangian L . Finally, we arrive at the total averaged Lagrangian,

$$L = N \left(\frac{3a^2 b_t}{2} - \frac{1}{2} \xi_t^2 + \varphi_t + \frac{3}{4a} + 3b^2 a^2 + \frac{2}{\sqrt{\pi} a^3} U_0 \xi^2 e^{-\frac{\xi^2}{a^2}} - \frac{3qN}{8\sqrt{2\pi}a} - \frac{gN}{4\sqrt{2\pi}} \frac{4w^2(a^2 + w^2) + 3a^4}{(a^2 + w^2)^{\frac{5}{2}}} \right). \quad (9)$$

The collective coordinate equations are derived from the averaged Lagrangian above. With q_i as the ansatz parameters of a, b, ξ, φ , we apply the Euler-Lagrangian equation below,

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{\Phi}_i} \right) - \frac{\partial L}{\partial q_i} = 0, \quad (10)$$

producing the following system of coupled equations for the two-soliton molecule parameters of the width and center-of-mass position,

$$a_{tt} = \frac{1}{a^3} - \frac{4U_0 \xi^2 e^{-\frac{\xi^2}{a^2}}}{3\sqrt{\pi}a^4} \left(\frac{2\xi^2}{a^2} - 3 \right) - \frac{qN}{4\sqrt{2\pi}a^2} + \frac{gN}{6\sqrt{2\pi}} F(a), \quad (11)$$

$$\xi_{tt} = -\frac{4U_0}{\sqrt{\pi}a^3} \xi e^{-\frac{\xi^2}{a^2}} \left(1 - \frac{\xi^2}{a^2} \right), \quad (12)$$

where

$$F(a) = \frac{(w^2 + a^2)(8a^2w + 12a^3 - 20aw^2) - 15a^5}{(w^2 + a^2)^{\frac{7}{2}}}. \quad (13)$$

Therefore, Eq. (11) and Eq. (12) are the main results of this VA method which provide insight into the scattering phenomena of the soliton molecule by external Delta potential. Both equations become decoupled when the external potential is absent, i.e., $U_0 = 0$ and the soliton molecule propagates freely with constant velocity and width. In particular, the stationary width a_s of the soliton molecule of the NLSE can be approximated from Eq. (11) by letting $a_{tt} = 0$ and there is no dipole-dipole interaction so that $g = 0$. The stationary width obtained is given by

$$a_s = \left(\frac{8\sqrt{2}}{qA^2} \right)^{\frac{1}{4}}. \quad (14)$$

This implies that the width may oscillate around this stationary point due to perturbation. On the other hand, the system becomes coupled when the soliton molecule approaches the external potential and the entire system of Eq. (11) - (12) should be taken into account. Afterward, Eq. (12) describes the scattering of the effective classical particle by a localized barrier such that

$$\xi_{tt} = -\frac{4U_0}{\sqrt{\pi}a^3} \xi e^{-\frac{\xi^2}{a^2}} \left(1 - \frac{\xi^2}{a^2} \right) = \frac{dV_p(\xi)}{d\xi}. \quad (15)$$

Integrating once the above equation reduces it into the following form,

$$\xi_t = -\frac{2U_0 \xi^2 e^{-\frac{\xi^2}{a^2}}}{\sqrt{\pi}a^3}, \quad (16)$$

which characterizes the velocity of the soliton molecule. The coupled equation of Eq. (11) and Eq. (12) are then interpreted numerically using different values of parameters in order to observe the behaviour of the two-soliton molecule interacted with external Delta potential. There are two

cases of observation were made, where the different potential strength and soliton's initial velocities were taken into account.

The interaction of two-soliton with different potential strength of Delta potential Eq. (4) and a constant velocity of $v_0 = 0.3$ can be referred to Figure 1. Figure 1 (above panel) illustrates that the two-soliton molecule reflects when it collides with a strong potential wall $V(x) = 3.0$. The two-soliton molecule happened to oscillate within the potential well for a while during the collision after $t = 10s$ until $t = 20s$ before it is reflected back from the potential of $V(x) = -3.0$ as shown in the Figure 1 (below panel). The width and amplitude of the solitons started to change when perturbation started to happen after it interacts with the potential barrier. Then, the two-soliton molecule maintained back its amplitude after the collision.

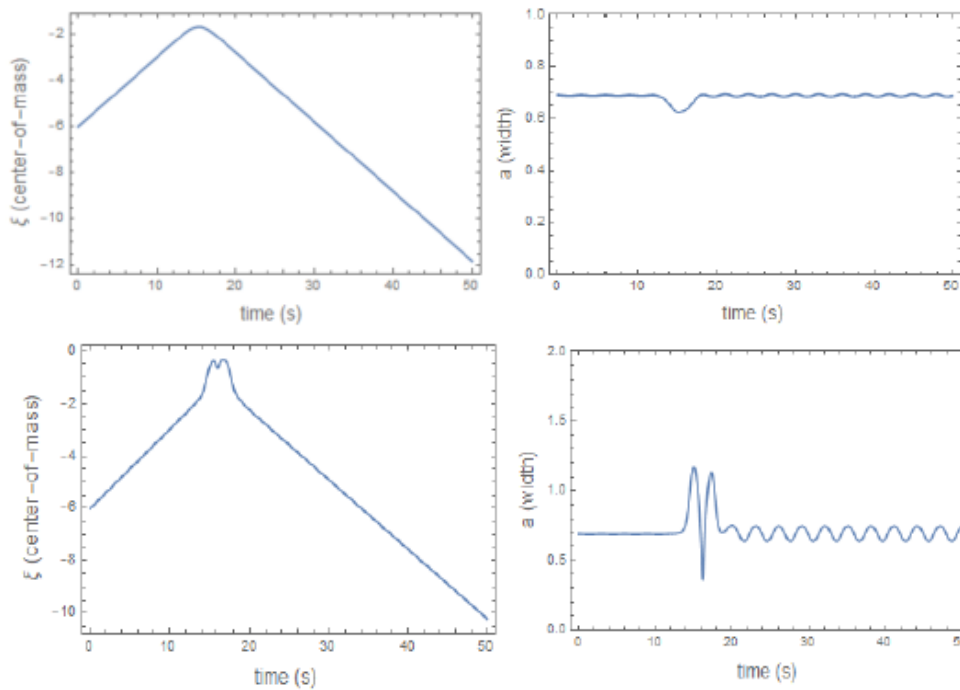


Figure 1: Evolution of the width and center of mass position of a soliton versus time t , according to ODE systems for Eq. (11) and (12). The parameters used are $v_0 = 0.3$, $V(x) = 3.0$ (above panel), $V(x) = -3.0$ (below panel).

In addition, Figure 2 shows the scattering of the two-soliton molecule by external Delta potential with different initial velocities of the soliton and similar potential strength of $V(x) = -3.0$. Figure 2 (above panel) shows that the two-soliton molecule moving with lower velocity is trapped and oscillates for a while within the potential well during the collision before a total reflection. The perturbation started to happen after $t = 6s$ when the amplitude and width started to change. On the other hand, Figure 2 (below panel) showed that with a higher value of soliton's initial velocity, the two-soliton molecule demonstrated a total transmission through the potential well after the collision with the barrier.

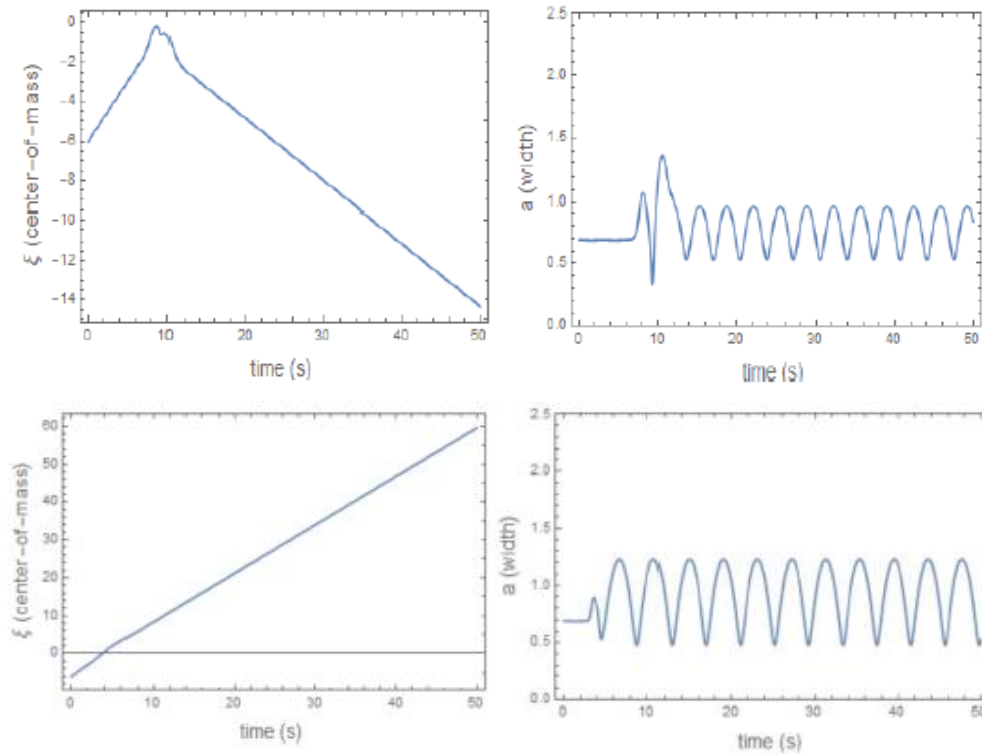


Figure 2: Evolution of the width and center of mass position of a soliton versus time t , according to ODE systems for Eq. (11) and (12). The parameters used are $V(x) = -3.0$, $v_0 = 0.6$ (above panel), $v_0 = 1.5$ (below panel).

DIRECT NUMERICAL SIMULATION

The VAM method is based on the assumption and describes an approximate result while direct numerical simulation shows an exact solution. The direct numerical simulation method of main Eq. (1) is used to verify the findings of the VAM method. In this method, the soliton is initiated with a certain velocity, v moving towards the potential barrier, $V(x)$ which is originally located far from the potential. In programming, there are two methods used which are Split Step Fourier Method (SSFM) and Fast Fourier Transform (FFT). Firstly, the first method is SSFM which is used to solve the time dependent nonlinear partial differential equation (PDE) and it followed by the old strategy where it divides and conquers (Suarez, 2015).

For the case of different potential strength, Figure 3 demonstrates the same outcomes when the two-soliton molecule scattered by the Delta potential wall, $V_0 = 3$ or potential well, $V_0 = -3$ where the initial velocity is fixed. Figure 3(a) illustrates the initial position of the two-soliton molecule before the interaction with the potential wall or well that is located at $x=0$. The two-soliton molecule then moves together towards the potential with the same velocity and the collision happened (see Figure 3(b) and Figure 3(c)). As the potential strength for both potential wall and well are strong enough to prevent the soliton molecule from passing through it, the two-soliton molecule is then reflected back to its original place, as shown in Figure 3(d), preserving its coherence as in Figure 3(e). The last figure shown in Figure 3 displays the summary of the movement of the two-soliton molecule towards the potential.

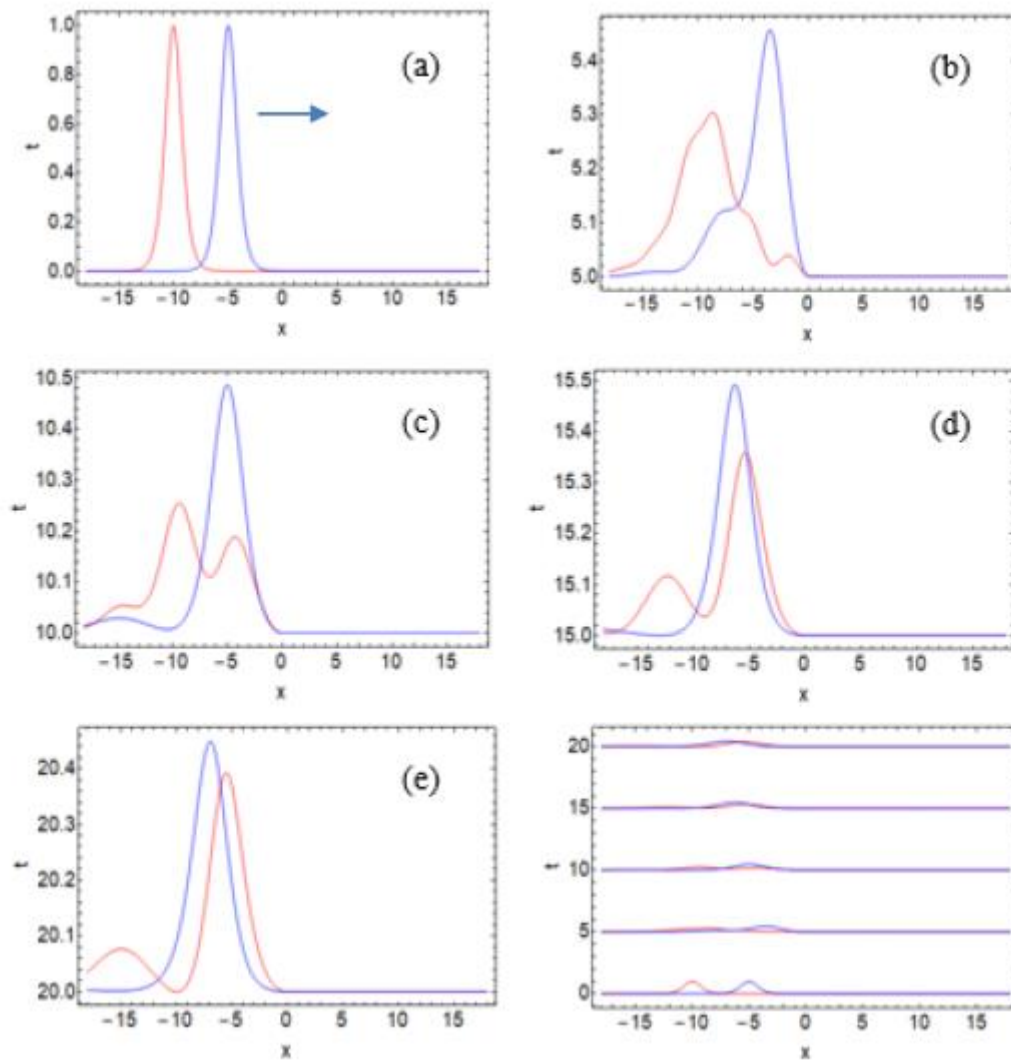


Figure 3: Evolution of the $|\psi_n|$ according to Eq. (1) and parameters used are the same as in Figure 1.

For the case of different soliton's initial velocities, the results for the scattering process when the two-soliton molecule moves with low and high velocities are depicted separately in Figure 4 and Figure 5. A fixed Delta potential well is considered for both examples where $V_0 = -3$ and the location is at $x=0$. At low velocity, $v_0 = 0.6$, the two-soliton molecule is reflected by the potential well as shown in Figure 4. Before the interaction, the soliton molecule propagates freely without being distorted as illustrated in Figure 4(a). When it approaches the potential well and starts to interact with it, the soliton molecule experiences perturbation (see Figure 4(b) and Figure 4(c)). Since the velocity is quite small, the two-soliton molecule cannot traverse through the strong potential well and therefore it is reflected back as shown in Figure 4(d) while conserving its coherence as in Figure 4(e). The last figure in Figure 4 summarizes the propagation of the two-soliton molecule towards the potential well.

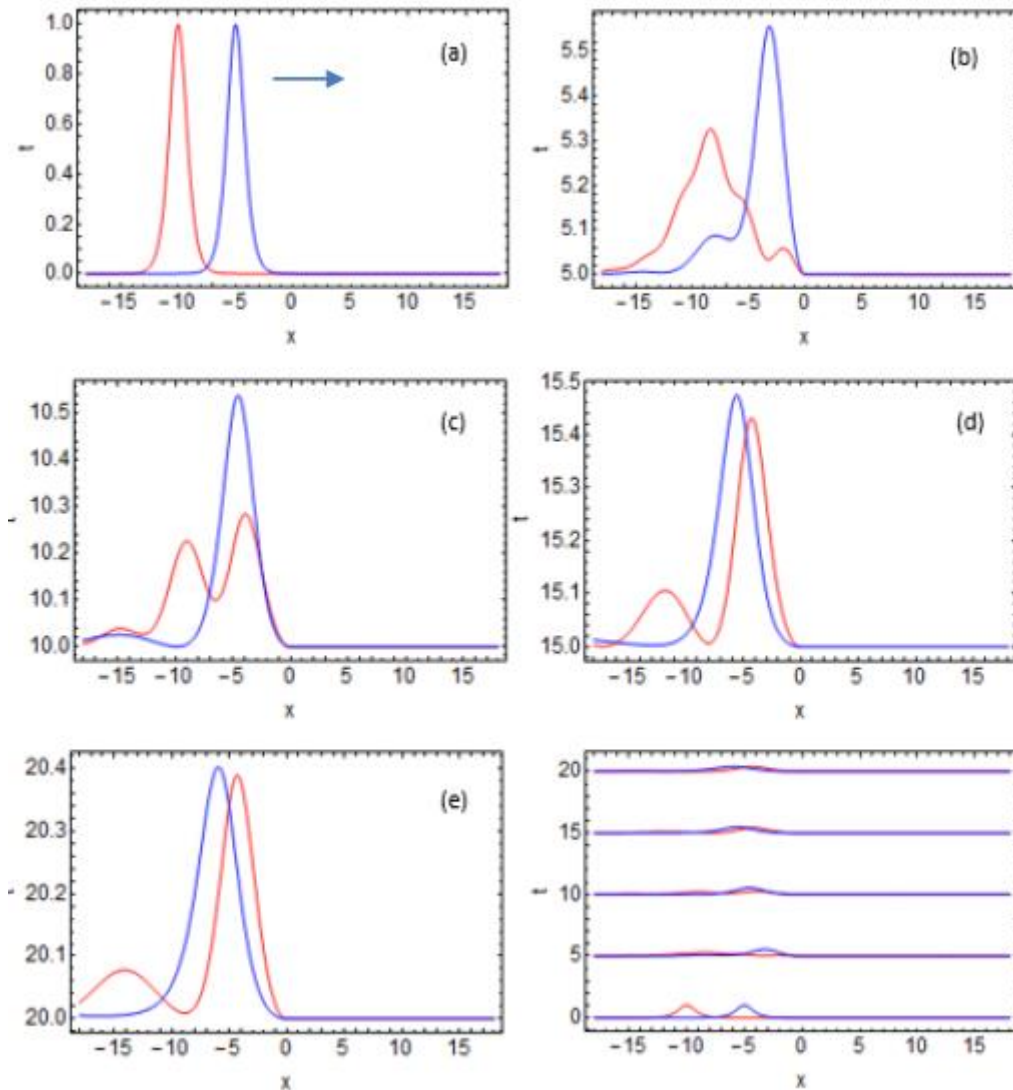


Figure 4: Evolution of the $|\psi_n|$ according to Eq. (1) and parameters used are the same as in Figure 2 (above panel).

On the other hand, the two-soliton molecule manages to transmit through the potential well when a high velocity, $v_0 = 1.5$ is considered as in Figure 5. At the beginning, Figure 5(a) shows that the two-soliton molecule moves constantly with unchanged shape when it is far away from the potential well. Then, collision with the potential well causes the shape of the two-soliton molecule starts to be disturbed as can be seen in Figure 5(b). Since the velocity is high, it has enough energy to travel through the potential well (see Figure 5(c) and Figure 5(d)). After that, the two-soliton molecule left the potential well behind and continues to move forward with higher velocity. The last picture in Figure 5 shows how the propagation and transmission of the two-soliton molecule occurs when interacting with the potential well. From both results, it indicates that the two-soliton molecule with a high velocity is able to propagate across the potential well, whereas it is reflected when it moves towards the potential with a low velocity.

Based on the results obtained from the numerical simulation using the governing equation of Eq. (1), it becomes apparent that the results confirm the behaviour of the two-soliton molecule as a classical particle in which it exhibits transmission or reflection when encountering the potential wall or well. Also, these results are quite similar to those obtained from the VAM

method, demonstrating the significance of the VAM method in describing the scattering behaviour of the two-soliton molecule under the influence of the external potential.

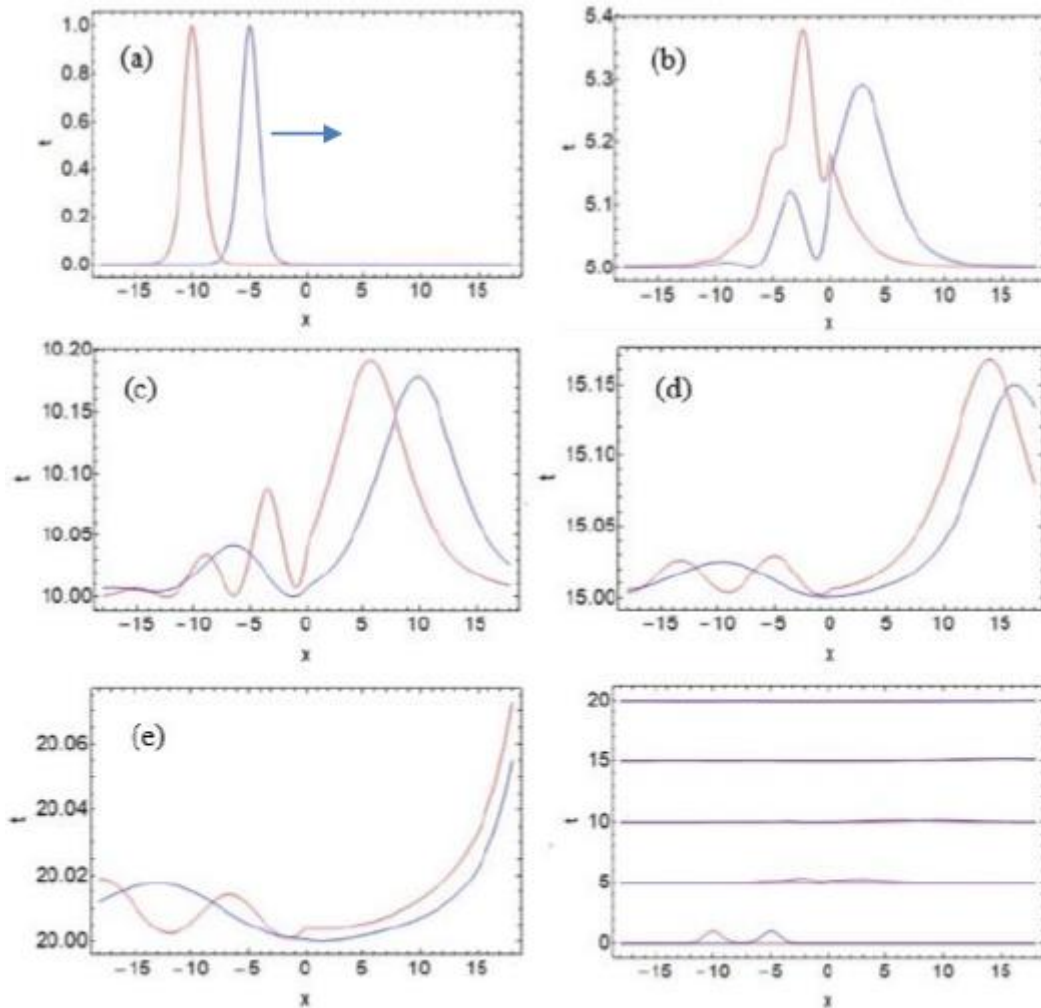


Figure 5: Evolution of the $|\psi_n|$ according to Eq. (1) and parameters used are the same as in Figure 2 (below panel).

CONCLUSION

This study mainly addressed how the behaviour of the two-soliton molecule nonlinear Schrödinger equation (NLSE) interacts with the external delta potential through analytical and numerical studies. This study also demonstrated how the two-soliton molecule behaves when it interacts with different potential strengths and soliton's initial velocities. In the case of different potential strengths, it exhibits the two-soliton molecule reflected back after colliding with the strong potential. In another case, given a different soliton's initial velocity, the two-soliton molecule is transmitted through the potential when it moves with a higher velocity, and it is reflected back when the velocity is low. For weak potentials and low velocity, the molecule preserves its coherence, meantime the internal modes are excited. At sufficiently low velocity of the incident molecule, we observe quantum reflection from the potential. Scattering by strong potentials at moderately high velocity ends up with dissociation of the molecule.

The VAM method shows results based on approximation and assumptions, while the direct numerical simulation of the main equation gives an exact solution. The direct numerical

simulation method is then used to verify the VAM results, and it appears that the outcomes from both methods were quite similar, which shows that strong correlation is attained between the results from both methods. The direct numerical simulation of the governing equation is a time-consuming method compared to the analytical analysis, or VAM method, which focuses more on analytical solutions and requires less time to solve the problem.

ACKNOWLEDGEMENT

This work has been supported by the project grant FRGS21-232-0841 of the International Islamic University of Malaysia.

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