

# Variational analysis of soliton scattering by external potentials

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**Abstract.** Dynamics of the width and center-of-mass position of a matter wave soliton subject to interaction with arbitrary external potential is analyzed using the collective coordinates approach. It is shown that approximation of the trial function and external potential only in the interaction region of the spatial domain is sufficient for adequate description of the soliton scattering process. The validity of the developed approach is illustrated for the Gaussian and Pöschl-Teller potentials.

## 1. Introduction

Soliton is a localized wave packet that can propagate in nonlinear media preserving its shape and velocity and exhibit particle like elastic collision with other solitons [1]. Theoretically studied and experimentally observed in different areas of physics, such as plasma physics, hydrodynamics, nonlinear optics, electric circuits, and more recently in Bose-Einstein condensates, solitons remain in the forefront of modern physics research [2]. Perhaps, the most important practical application of solitons to date pertains to information transfer through optical fibers [3]. Over the years enhancing the capacity of optical fiber communication systems employing solitons as information bit carriers has been the strongest motivation for scientific and engineering efforts in this field [4, 5].

Solitons in Bose-Einstein condensates present a promising candidate system for applications in high precision devices, such as atom interferometers [6], and studies of atom-surface interfaces [7]. A central mechanism here is the coherent interaction of the bright matter wave soliton with a potential barrier or well. The possibility to split the soliton through scattering on a Gaussian barrier with subsequent recombining the fragments was demonstrated in the recent experiment [8]. Theoretical analysis of the experiment and related process of soliton molecule formation was reported in [9].

Variational approximation, also known as the collective coordinates approach, is widely employed theoretical tool for the analysis of non-integrable soliton bearing equations [10, 11]. The success of the variational approximation critically depends of the proper choice of the trial function. The decisive point here is that, analytical evaluation of the averaged/effective Lagrangian should have been possible to obtain the system of evolution equations for the



parameters of the soliton. The choice of the Gaussian profile as a trial function is frequently found in the literature, because it suits the above mentioned purpose in many cases. However, in the matter wave soliton scattering processes under investigation, the Gaussian initial profile gives rise to a breathing wave packet. Moreover, the motion of the packet is accompanied by shedding linear waves, since the Gaussian is not the exact solution to the governing equation without external potential. Both of these processes, breathing motion of the soliton before the scattering and radiation of linear waves, are irrelevant and must be avoided. A possible way around this difficulty is adopting a trial function belonging to the soliton family, and replacing it by an equivalent Gaussian function *only* in the interaction region of the spatial domain. Then the corresponding term of the averaged Lagrangian can be evaluated exactly. Efficiency of this method was demonstrated in [12] for propagation of solitons in liquid crystals.

In the variational approximation developed below we assume the trial function to be of the hyperbolic secant function with time dependent parameters. While the soliton is far away from the scattering potential the interaction between them is effectively zero, and one has a freely propagating matter wave packet with constant parameters, such as the amplitude, width, center-of-mass position and velocity. Time dependence of the parameters become evident when the soliton starts to interact with the potential, namely it experiences deformation and changes velocity. Perturbation of the soliton in the form of oscillating amplitude and width remains long after the interaction. This process is interpreted as excitation of soliton's internal modes. Frequency of oscillations can be estimated from variational equations, as illustration of the predictive power of the variational approach.

The paper is organized as follows. In Sec. II the mathematical model is formulated and basic equations are derived. Sec. III is devoted to numerical simulations of the variational equations and comparison of the results with direct solution of the original Gross-Pitaevskii equation. Finally, in Sec. IV we summarize our findings, and discuss some interesting directions for future studies.

## 2. The model and main equations

The model is based on the reduced nonlinear Schrödinger/Gross-Pitaevskii equation (GPE)

$$i\psi_t + \frac{1}{2}\psi_{xx} - V(x)\psi + g|\psi|^2\psi = 0, \quad (1)$$

where  $\psi(x, t)$  is the macroscopic wave function of the quasi-one dimensional condensate,  $V(x)$  is the external potential. We consider positive coefficient of nonlinearity ( $g > 0$ ), which corresponds to attractive interactions between atoms in the condensate, or focusing nonlinearity in optics applications. In absence of external potential ( $V(x) = 0$ ) and  $g = 1$  the Eq. (1) possesses fundamental bright soliton solution

$$\psi(x, t) = A \operatorname{sech}[A(x - \xi(t))] \exp(i\Theta), \quad \Theta(x, t) = \frac{1}{2}(A^2 - \xi^2)t + vx + \varphi, \quad v = \xi_t, \quad (2)$$

where  $A, \xi, v, \varphi$  are the amplitude, center of mass position, velocity and phase of the soliton respectively. Trial function of the variational approximation will be assumed to be of this form. This means that the shape of the soliton remains close to the shape of hyperbolic secant function, although its amplitude and width may change significantly during the whole period of evolution.

It is easy to verify that the governing Eq. (1) can be obtained from the following Lagrangian density

$$\mathcal{L} = \frac{i}{2}(\psi\psi_t^* - \psi^*\psi_t) + \frac{1}{2}|\psi_x|^2 + V(x)|\psi|^2 - \frac{g}{2}|\psi|^4, \quad (3)$$

by means of the Euler-Lagrange equation. Spatial integration of the Lagrangian density  $L = \int_{-\infty}^{\infty} \mathcal{L} dx$  using the trial function

$$\psi(x, t) = A \operatorname{sech} \left( \frac{x - \xi}{a} \right) e^{ib(x-\xi)^2 + iv(x-\xi) + i\varphi}, \quad (4)$$

gives rise to following averaged/effective Lagrangian

$$L = N \left[ \frac{\pi^2}{12} a^2 b_t + \frac{\pi^2}{6} a^2 b^2 - \frac{1}{2} \xi_t^2 + \varphi_t + \frac{1}{6a^2} - \frac{gN}{6a} + \frac{1}{2a} \int_{-\infty}^{\infty} V(x) \operatorname{sech}^2 \left( \frac{x - \xi}{a} \right) dx \right]. \quad (5)$$

The norm of the wave function  $N = \int_{-\infty}^{\infty} |\psi|^2 dx = 2A^2 a$  is proportional to the number of atoms in the condensate and represents a conserved quantity.

Evolution equations for variational parameters can be derived from the Euler-Lagrange equations  $d/dt(\partial L/\partial \dot{q}_i) - \partial L/\partial q_i = 0$ , where  $q_i$  are time dependent collective coordinates  $a, \xi, b, \varphi$ . The equation for the phase  $\varphi$  reduces to  $dN/dt = 0$  and illustrates the conservation of the norm of the wave function or number of atoms in the condensate. It is decoupled from other equations and can be dropped in further analysis. What remains is a set of coupled equations for the width and center-of-mass position of the soliton

$$a_{tt} = \frac{4}{\pi^2 a^3} - \frac{2gN}{\pi^2 a^2} + \frac{6}{\pi^2 a^2} F_1(V, a, \xi), \quad (6)$$

$$\xi_{tt} = -\frac{1}{a^2} F_2(V, a, \xi), \quad (7)$$

where

$$F_1(V, a, \xi) = \int_{-\infty}^{\infty} V(x) \operatorname{sech}^2 \left( \frac{x - \xi}{a} \right) \left[ 1 - \frac{2(x - \xi)}{a} \operatorname{th} \left( \frac{x - \xi}{a} \right) \right] dx,$$

$$F_2(V, a, \xi) = \int_{-\infty}^{\infty} V(x) \operatorname{sech}^2 \left( \frac{x - \xi}{a} \right) \operatorname{th} \left( \frac{x - \xi}{a} \right) dx.$$

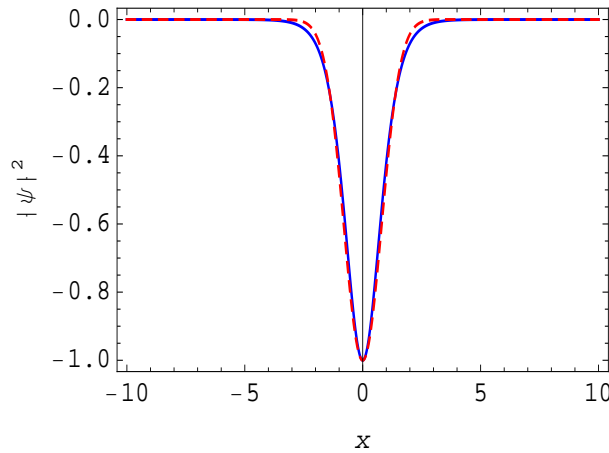
The coupled system of dynamical equations (6)-(7) for description of soliton scattering by arbitrary external potential  $V(x)$  is the main result of this work. Here it is necessary to note that the last term in effective Lagrangian (5) cannot be calculated analytically for arbitrary potentials  $V(x)$ , therefore Eqs. (6)-(7) are the integro-differential equations. Available integration routines [13, 14] provide fast and high precision numerical simulations for both the GPE (1) and variational (6)-(7) equations.

However, before proceeding to numerical simulations we present analytical approximations for the integral in Eq.(5) to enhance the efficiency of the developed method. Similar technique was reported in [15] where a deep and narrow Pöschl-Teller potential was replaced by the Dirac delta function  $V(x) = V_0 \delta(x)$ . Below we consider another case when both the potential and wave function can be approximated by Gaussian functions.

$$V(x) \rightarrow V_0 \exp(-x^2/w^2), \quad \operatorname{sech}^2 [(x - \xi)/a] \rightarrow \exp \left[ -(x - \xi)^2/a^2 \beta^2 \right], \quad (8)$$

where  $w$  is the width of the potential, and  $\beta = 2/\sqrt{\pi}$  is found from the requirement of equal areas beneath the curves

$$\int_{-\infty}^{\infty} \operatorname{sech}^2 \left( \frac{x}{a} \right) dx = \int_{-\infty}^{\infty} \exp \left( -\frac{x^2}{\beta^2 a^2} \right) dx. \quad (9)$$



**Figure 1.** Comparison of the Gaussian (blue solid line) and hyperbolic secant (red dashed line) functions of equal norms as illustration for the approximation (8). Parameters:  $V_0 = -1$ ,  $a = 1$ ,  $\beta = 2/\sqrt{\pi}$ ,  $\xi = 0$ .

The accuracy of the approximation (8) is illustrated in Fig. 1. Now the integrals in Eq. (5) can be readily calculated with Gaussian functions and the effective Lagrangian (5) takes the form

$$L = N \left[ \frac{\pi^2}{12} a^2 b_t + \frac{\pi^2}{6} a^2 b^2 - \frac{1}{2} \xi_t^2 + \varphi_t + \frac{1}{6a^2} - \frac{gN}{6a} + V_0 \frac{w}{\beta(\beta^2 a^2 + w^2)^{1/2}} \exp\left(-\frac{\xi^2}{\beta^2 a^2 + w^2}\right) \right].$$

Corresponding dynamical equations for the width and center-of-mass position read as follows

$$a_{tt} = \frac{4}{\pi^2 a^3} - \frac{2gN}{\pi^2 a^2} - V_0 \frac{12\beta a w (2\xi^2 - \beta^2 a^2 - w^2)}{\pi^2 (\beta^2 a^2 + w^2)^{5/2}} \exp\left(-\frac{\xi^2}{\beta^2 a^2 + w^2}\right), \quad (10)$$

$$\xi_{tt} = V_0 \frac{2w\xi}{(\beta^2 a^2 + w^2)^{3/2}} \exp\left(-\frac{\xi^2}{\beta^2 a^2 + w^2}\right), \quad (11)$$

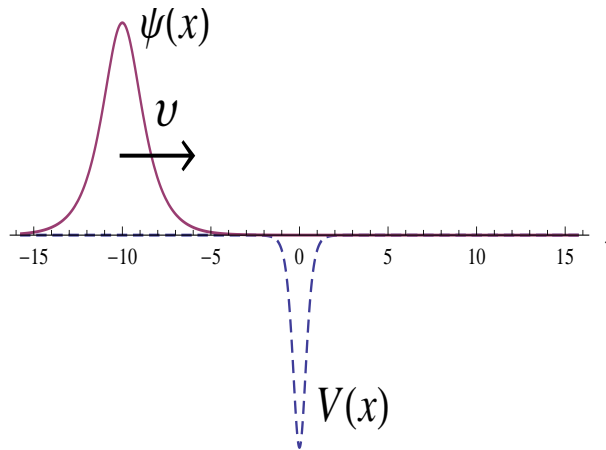
If the scattering potential also has the form  $\sim \text{sech}^2(x/w)$ , one should substitute  $w \rightarrow \beta w$  in these equations. In the next section we compare predictions of exact (6)-(7) and approximate (10)-(11) variational equations with the numerical solution of the original GPE (1).

### 3. Numerical simulations

Numerical solution of the GPE (1) has been performed by the split-step fast Fourier transform method [16] using 2048 Fourier modes within the integration domain of length  $L \in [-50 \div 50]$ , and the time step was  $\delta t = 0.005$ . Accuracy of calculations was monitored through conserved quantities of the governing equation. In particular the norm of the wave function was constant with tolerance  $\sim 10^{-3}$  through the whole period of evolution. To avoid the adverse effect of linear waves emitted by the soliton during scattering on the potential, we installed absorbing boundary layers at both ends of the integration domain as described in [17]. This technique emulates the condition of infinite spatial domain for the GPE (1).

The dynamical equations of the variational approximation (6)-(7) and (10)-(11) are solved using the Runge-Kutta procedure of 5-th order with adaptive step-size control [13]. Fast evaluation of the integral terms  $F_1(V, a, \xi)$ ,  $F_2(V, a, \xi)$  in Eq. (6)-(7) are performed by adaptive Newton-Cotes integration routine, based on eighth-degree polynomial [14].

Arrangement for the soliton scattering by external potential well/barrier is depicted in Fig. 2. Soliton  $\psi(x)$  is set in motion with some velocity  $v$  towards the potential well/barrier  $V(x)$  initially located at some distance from it. Depending on the parameters of the problem soliton is either reflected or transmitted through the potential. We monitor the evolution of the width



**Figure 2.** Schematic view for the soliton scattering in numerical experiments.

and center-of-mass position of the soliton via numerical solution of the GPE and variational equations

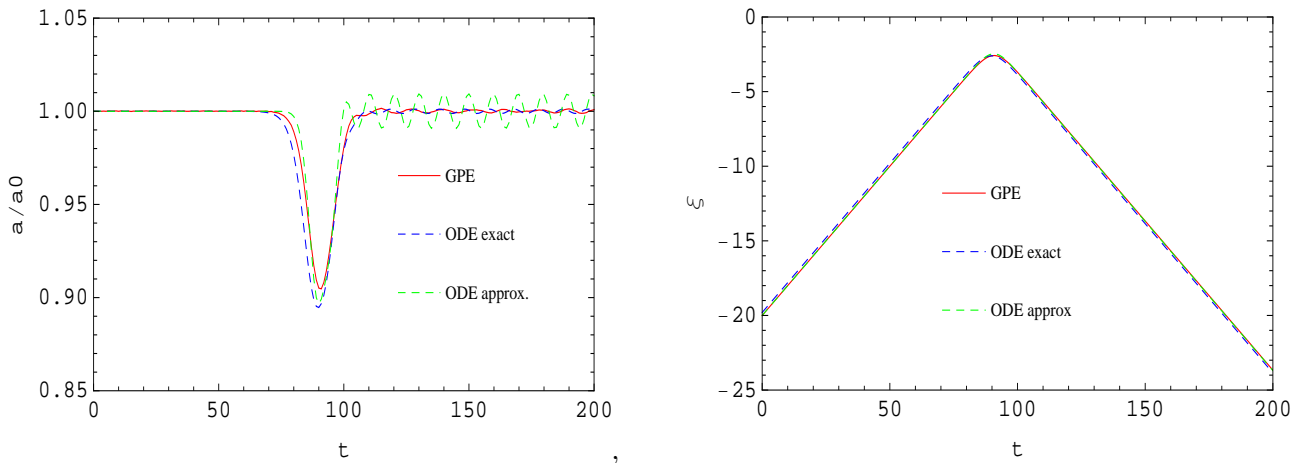
$$\xi(t) = \frac{\int_{-\infty}^{\infty} x |\psi(x, t)|^2 dx}{\int_{-\infty}^{\infty} |\psi(x, t)|^2 dx}, \quad a(t) = \left( \frac{12}{\pi^2} \cdot \frac{\int_{-\infty}^{\infty} (x - \xi(t))^2 |\psi(x, t)|^2 dx}{\int_{-\infty}^{\infty} |\psi(x, t)|^2 dx} \right)^{1/2}.$$

### 3.1. Scattering on the Gaussian potential

First we consider the scattering of a matter wave soliton by a Gaussian potential barrier and well. In experiments with Bose-Einstein condensates the potential barrier/well for neutral atoms is created using a laser beam, whose frequency  $\omega$  is slightly shifted from the frequency  $\omega_0$  of atomic transitions [18]. The mechanism is based on the dipole force exerted on an atom by an inhomogeneous light field. If the difference  $\Delta = \omega - \omega_0$  is negative ( $\Delta < 0$ , red detuning) the dipole potential is attractive and the atoms are pulled towards the maximum of the laser light intensity. In this case the laser beam acts as a potential well for the atomic wave packet. Similarly, blue detuned ( $\Delta > 0$ ) laser beam acts as a potential barrier for matter wave solitons.

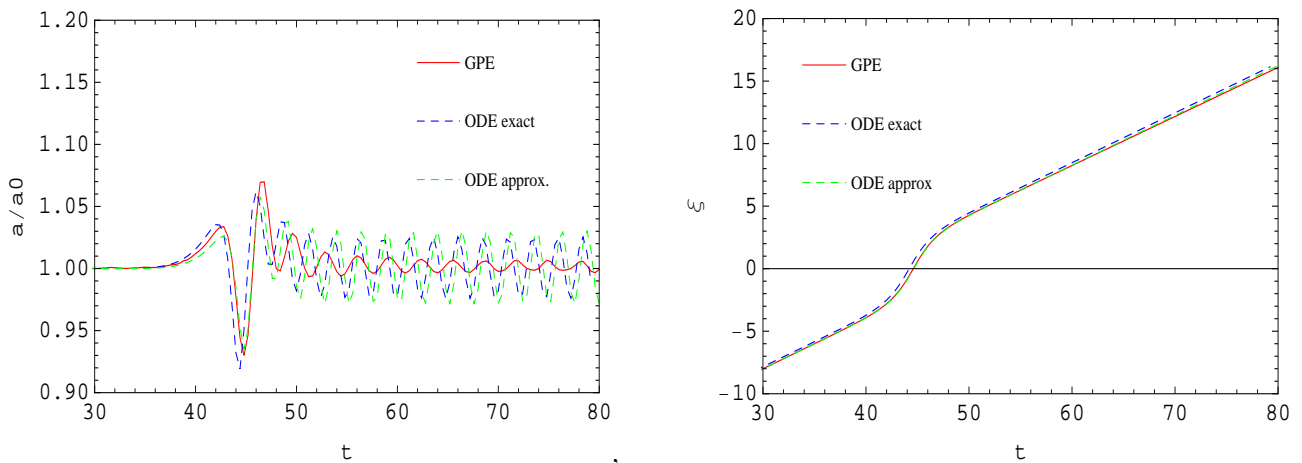
In Fig. 3 the scattering of a soliton by a Gaussian potential barrier is shown through the time dependence of its relative width and center-of-mass trajectory. The soliton at initial position  $\xi_0$  is set in motion, with velocity  $v$ , towards the potential barrier at the origin. Until the soliton reaches the interaction range of the potential barrier  $\sim w$ , it moves freely with constant width and velocity. Reflecting barrier forces the soliton to shrink and expand again, reversing the direction of its motion. As can be seen from the figure, dynamical equations of the variational approximation (6)-(7) and (10)-(11) provide fairly good description of the scattering process, when compared with direct numerical solution of the original GPE (1).

Scattering of the soliton on the potential well is quite different from the previous case of a barrier. Excitation of bound states of the well by approaching matter wave packet is the influential process in this case, because the outcome of the soliton scattering strongly depends on the nature of this interaction, i.e. whether it is repulsive or attractive. In fact, when the bound states of the potential well are excited, the single soliton trial function (4) of the variational approximation becomes inaccurate (see also the next subsection).



**Figure 3.** Evolution of the width and center-of-mass position of a soliton  $\psi(x,0) = \text{Asech}[(x - \xi_0)/a] \exp(-vx)$  reflected by a Gaussian potential barrier  $V(x) = V_0 \exp(-x^2/w^2)$ , according to GPE and ODE systems: (6)-(7) - exact, (10)-(11) - approximate. Left panel: At the impact upon the potential barrier soliton shrinks and expands, but small amplitude oscillations remain after the collision. Right panel: Center-of-mass dynamics is perfectly reproduced by the variational approximation. Parameters:  $V_0 = 0.5$ ,  $w = 1$ ,  $A = 1$ ,  $a = 1$ ,  $v = 0.2$ ,  $\xi_0 = -20$ .

In numerical simulations presented below we consider a wave packet which is narrow and tall compared with the extent and strength of the well. In this case the leakage of matter from the wave packet and excitation of the bound states in the well, are inhibited. Fig. 4 illustrates typical example of soliton scattering by Gaussian potential well.



**Figure 4.** Time dependence of the width and center-of-mass position of the soliton with  $A = 2$ ,  $a = 0.5$ ,  $v = 0.4$ ,  $\xi_0 = -20$ , transmitted through a Gaussian potential well with  $V_0 = -1$ ,  $w = 2$  according to GPE and ODE systems: (6)-(7) - exact, (10)-(11) - approximate. Left panel: In the spatial domain of the potential soliton exhibits strong variations of the width, which transforms into steady oscillations after the interaction. Therefore, traversing the potential well leads to excitation of internal modes of the soliton. Right panel: As in the case of the barrier, center-of-mass dynamics is described very well by both versions of the variational approximation.

A noteworthy feature of the scattering process shown in the right panel of Fig. 4 is the

accelerated motion of the soliton within the spatial domain of the potential well (at  $t \sim 40 \div 50$ ). This phenomenon, called "time advance" effect, was first shown for a linear wave packet passing over the reflectionless potential [19], and later reported for solitons traversing the Pöschl-Teller potential [15]. Here we observe the same effect in the numerical simulations of the soliton scattering by a Gaussian potential well. As in the above mentioned cases, on leaving the interaction region the soliton restores its original velocity possessed before the scattering event.

### 3.2. Scattering on the Pöschl-Teller potential

The Pöschl-Teller potential

$$V(x) = -\frac{\hbar^2}{2mw^2} \frac{\nu(\nu + 1)}{\cosh^2(x/w)} \quad (12)$$

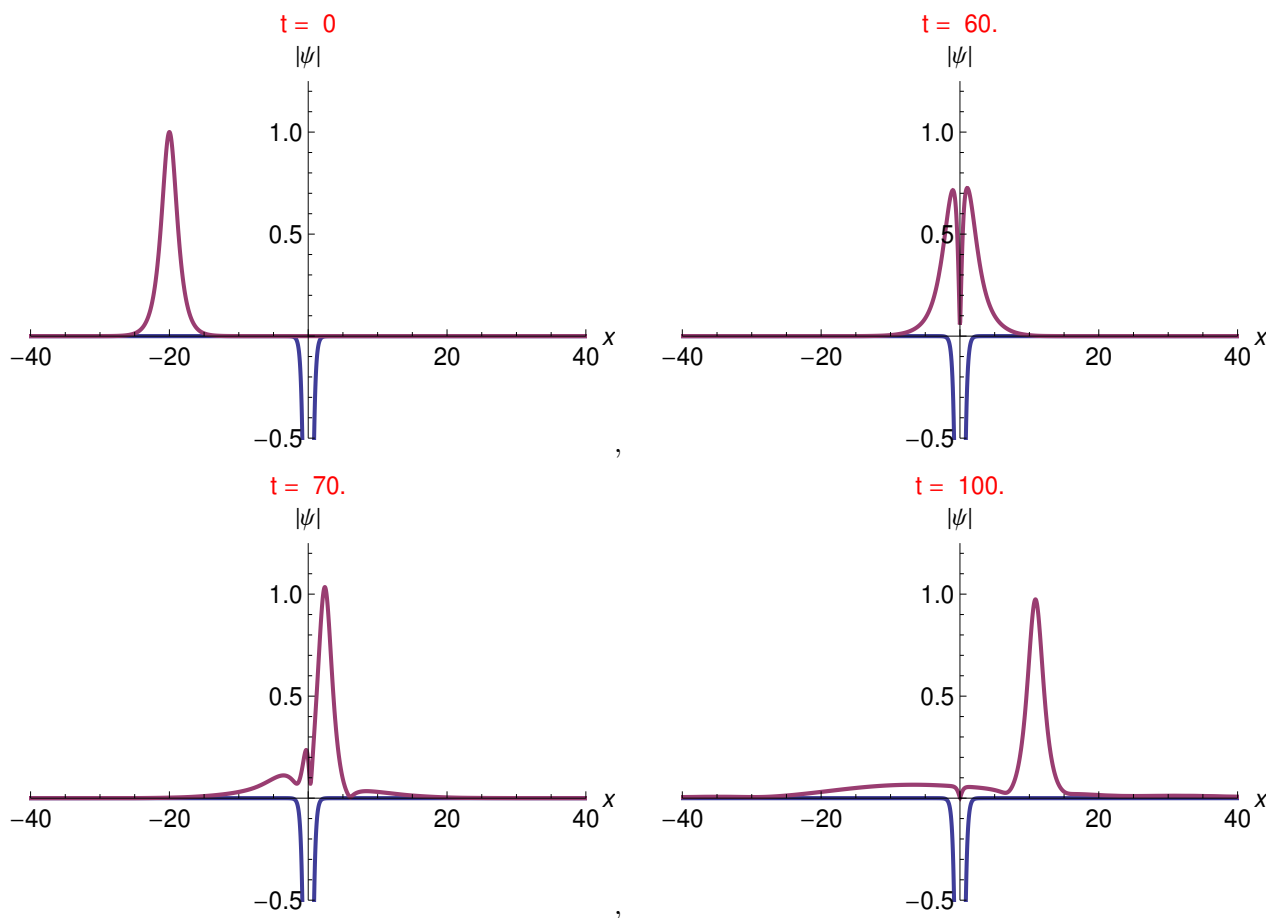
has a remarkable property of being fully transparent for linear waves with arbitrary energy, if  $\nu$  is a positive integer [20]. The absence of reflected waves at any energy, when the dielectric function profile possesses the form (12), has found practical applications in the design of optical coatings permitting the uninterrupted passage of light [21].

Recently it was revealed that the potential (12) exhibits peculiar features also in the interactions with nonlinear waves. Namely, if the soliton approaches the potential well at velocity less than some critical value, it is almost fully reflected. By contrast, solitons with velocity higher than critical, are almost fully transmitted [22]. Particularly, for the potential  $V(x) = V_0/\cosh^2(x/w)$  with  $V_0 = -4, w = 0.5$ , the critical velocity was found to be  $v_{cr} = 0.325$  [22]. Similar behavior was observed in the scattering of soliton molecules as well [15]. Matter wave soliton approaching the Pöschl-Teller potential well excites quantum bound states of the well. Interaction of the soliton with emerging localized states in the potential well crucially influences the process of scattering. That is why here the variational approximation with the single component trial function fails, as can be inferred from Fig. 5. The possibility of taking into account the bound states of the well in the collective coordinate approach was considered in Refs. [23, 22], but for the delta function case and without comparison with GPE. Below we provide such comparison for the case of the weak potential well.

In Fig. 6 the results for soliton scattering on the shallow potential (12) is presented. Predictions of the variational approach are compared with the results of direct numerical solution of the GPE (1). As can be admitted, the coupled set of variational equations provide qualitatively correct description for the evolution of the soliton's width and center-of-mass dynamics. One peculiarity to be noted here is that the reflected soliton (middle panel) performs breathing oscillations with less amplitude ( $\sim 3\%$  of stationary value) than the transmitted one ( $\sim 40\%$ ). In both cases the variational approximation overestimates the amplitude of oscillations. However, the frequencies of oscillations are in good agreement.

## 4. Conclusions

We have developed a variational approximation to describe the scattering of matter wave solitons by external potentials of arbitrary shape. Dynamical equations for the parameters of the soliton have the form of integro-differential equations. The possibility to solve these equations quickly and accurately, using standard numerical procedures, has been demonstrated. Quite good agreement between the results of variational equations and direct numerical solution of the original Gross-Pitaevskii equation is found for soliton scattering on potential barriers, while scattering on potential wells is described qualitatively. The proposed approach can be extended to other soliton bearing equations, such as generalized nonlinear Schrödinger equation and nonlocal Gross-Pitaevskii equation for dipolar condensates. The results can be useful in development of new methods aimed at probing the external potentials/defects by scattering solitons on them.

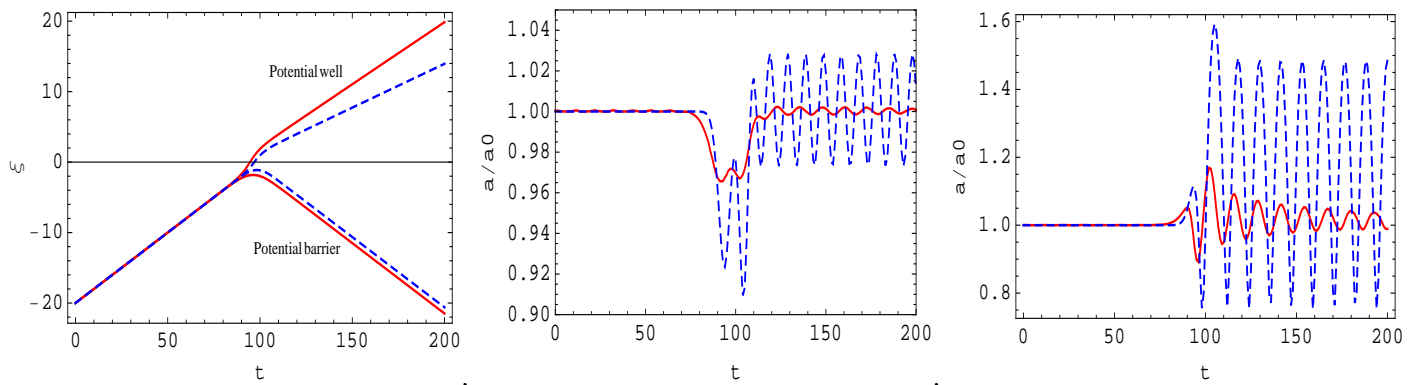


**Figure 5.** Transmission of the soliton with  $A = 1$ ,  $a = 1$ ,  $\xi_0 = -20$  through the potential well  $V(x) = V_0/\cosh^2(x/w)$ , with  $V_0 = -4$ ,  $w = 0.5$  at slightly overcritical velocity  $v = 0.35$ . Strong deformation of the soliton in the interaction region implies that the variational approximation with the trial function (4) will fail in this case. For visual convenience only the upper part of the potential is shown (blue line).

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**Figure 6.** Reflection/transmission of the matter wave soliton with  $A = 1, a = 1, v = 0.2$ , through a shallow potential barrier/well  $V(x) = V_0/\cosh^2(x/w)$  with  $V_0 = \pm 0.1, w = 1$ . Red solid and blue dashed lines correspond to numerical solution of the GPE (1) and predictions of the variational equations (10)-(11). Left panel: Center-of-mass dynamics. Middle and right panels: Dynamics of the width for potential barrier and well respectively

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