Scattering of a two-soliton molecule by Gaussian potential barriers and wells

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Abstract. Two anti-phase bright solitons in a dipolar Bose-Einstein condensate can form stable bound states, known as soliton molecules. In this paper we study the scattering of a two-soliton molecule by external potential, using the simplest and analytically tractable Gaussian potential barriers and wells, in one spatial dimension. Theoretical model is based on the variational approximation for the nonlocal Gross-Pitaevskii equation (GPE). At sufficiently low velocity of the incident molecule we observe quantum reflection from the potential well. Predictions of the mathematical model are compared with numerical simulations of the GPE, and good qualitative agreement between them is demonstrated.

1. Introduction

Manifestation of quantum behavior by macroscopic objects always attracts great interest. One of the recent findings in this direction has been the observation of quantum reflection of matter-wave solitons from attractive potential wells and downward potential steps [1, 2, 3]. Experimental study of the quantum reflection of a matter-wave soliton, formed from ^{85}Rb Bose-Einstein condensate, was reported in [4]. In the present context, the quantum reflection is understood as a classically forbidden reflection, because it occurs without reaching the classical turning point.

Gaining new knowledge by studying collisions of particles with each-other, or their interaction with external potentials, represents the leading approach in particle physics. Similar method is applicable in studies of nonlinear localized wave packets or solitons. By definition, solitons are robust localized wave packets, that can propagate along wave-guides preserving their shape and velocity. Solitons emerge from a fine balance between dispersive spreading and nonlinear self focusing of the wave packet. During the interactions solitons exhibit both particle-like and wave-like properties. In particular, two colliding solitons exchange not only their velocities, as classical particles do, but also their physical locations, as quantum particles do via the tunnel phenomenon. Experimental demonstration [5] and theoretical confirmation [6] of the last property has been a significant achievement in the physics of solitons. The discovery of stable bound states of optical solitons, known as soliton molecules [7, 8, 9], represents another significant advance in the field. Recently the existence of similar soliton complexes in dipolar Bose-Einstein condensates was reported in [10, 11].

In this work we study the scattering of a soliton molecule by potential barriers and wells to find out, whether the quantum reflection is observed in such a setting. Of particular interest is the excitation of internal modes of soliton molecules, as a result of scattering process. We address the problem using the analytical methods and numerical simulations. The analytical method is based on the variational approximation, which is briefly described below.

2. The model and variational approach

The governing equation of our model is the one-dimensional nonlocal Gross-Pitaevskii equation (GPE), which in dimensionless units has the following form

$$i\frac{\partial\psi}{\partial t}+\frac{1}{2}\frac{\partial^2\psi}{\partial x^2}-V(x)\psi+q|\psi|^2\psi+g\psi\int\limits_{-\infty}^{+\infty}R(|x-\xi|)\,|\psi(\xi,t)|^2d\xi=0, \tag{1}$$

where $\psi(x,t)$ is the mean-field wave function of the condensate, $V(x)$ is the external potential, q and g are, respectively, the coefficients of nonlinearity, responsible for the short-range contact and long-range dipole-dipole interactions between atoms in the condensate. The wave function is normalized to the reduced number of atoms in the condensate $N=\int_{-\infty}^{+\infty}|\psi(x)|^2dx$, which is a conserved quantity of Eq. (1). The response function $R(x)$ characterizes the degree of non-locality of the medium. It shows how strongly the properties of the medium at given location depends on the properties at neighboring regions. For the contact interactions, when the particles influence each-other only when they are at the same spatial point, the response function is equal to the Dirac delta function. For the long-range dipole-dipole interactions, we approximate the response function by a Gaussian

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

which is normalized to one $\int_{-\infty}^{+\infty}R(x)dx=1$. This response function is simple for analytical treatment and sufficient for understanding of the problem at hand. In fact $R(x)$ is qualitatively similar to the response function, obtained from rigorous calculations [12].

To develop the variational approximation (VA) we note that the governing GPE (1) can be generated from the following Lagrangian density

$$\mathcal{L}=\frac{i}{2}(\psi\psi_t^*-\psi^*\psi_t)+\frac{1}{2}|\psi_x|^2+V(x)|\psi|^2-\frac{1}{2}q|\psi|^4-\frac{1}{2}g|\psi(x,t)|^2\int\limits_{-\infty}^{\infty}R(x-\xi)|\psi(\xi,t)|^2d\xi. \tag{3}$$

An important step in development of the VA is selection of suitable trial function. As a trial function for the two-soliton molecule we use the first Gauss-Hermite function [13, 14, 15]

$$\psi(x,t)=A(t)\cdot(x-\xi)\cdot\exp\left[-\frac{(x-\xi)^2}{2a(t)^2}+ib(t)(x-\xi)^2+iv(t)(x-\xi)+i\phi(t)\right], \tag{4}$$

where $A(t),a(t),b(t),v(t),\phi(t)$ are time-dependent variational parameters, meaning the amplitude, width, chirp parameter, velocity and phase of the soliton molecule, respectively. The velocity is defined as a time derivative of the molecule's center-of-mass position $v=\xi_t$. The norm $N=A^2a^3\sqrt{\pi}/2$, which is a conserved quantity of the governing equation, is proportional to the number of atoms in the condensate. In fact the waveform (4) can be approximated quite accurately by two anti-phase Gaussian functions (single solitons). The spatial separation between two soltion's center-of-mass positions (molecular bond length) is

defined as $\Delta = 4a/\sqrt{\pi}$. Below we consider the Gaussian $V(x) = V_0 \cdot \exp\left[-x^2/(2d^2)\right]$ and Pöschl-Teller $V(x) = V_0 \cdot \mathrm{sech}^2(\alpha x)$ potentials as examples. For $V_0 > 0$ we have the potential barrier, while $V_0 < 0$ corresponds to the potential well.

Now using the response function (2) and ansatz (4), we evaluate the Lagrangian density (3). Subsequent integration over the space variable $L = \int \mathcal{L} dx$ yields the averaged Lagrangian

$$\frac{L}{N} = \frac{3}{2}a^2 b_t - \frac{1}{2}\xi_t^2 + \phi_t + \frac{3}{4a^2} + 3\,a^2 b^2 - \frac{3qN}{8\sqrt{2\pi}a} - \frac{gN}{8\sqrt{2\pi}}F(a) + 2\sqrt{2}V_0 d G(a,\xi), \tag{5}$$

where

$$F(a) = \frac{4w^2(w^2+a^2)+3a^4}{(w^2+a^2)^{5/2}}, \quad G(a,\xi) = \frac{d^2(a^2+2d^2)+a^2\xi^2}{(a^2+2d^2)^{5/2}} \exp\left(-\frac{\xi^2}{a^2+2d^2}\right).$$

In the case of a Pöschl-Teller potential the hyperbolic secant can be approximated by a Gaussian function $\mathrm{sech}^2(\alpha x) \simeq \exp(-\pi\alpha^2 x^2/4)$, which was shown to be quite accurate [16]. Therefore, for the Pöschl-Teller potential in the above and subsequent equations we can substitute $d = \sqrt{2/\pi}/\alpha$.

The Euler-Lagrange equations $d/dt(\partial L/\partial \nu_t) - \partial L/\partial \nu = 0$ for variational parameters $\nu \to a,\ b,\ \xi,\ \phi$ give the following coupled system for the width and center-of-mass position of the soliton molecule

$$a_{tt} = \frac{1}{a^3} - \frac{qN}{4\sqrt{2\pi}a^2} - \frac{gN}{4\sqrt{2\pi}} \cdot \frac{a(a^4+4w^4)}{(a^2+w^2)^{7/2}} - \frac{4\sqrt{2}V_0 d}{3} \cdot \frac{\partial G(a,\xi)}{\partial a}, \tag{6}$$

$$\xi_{tt} = -4\sqrt{2}V_0 d\,\xi \cdot \frac{a^4 + a^2(d^2-\xi^2) - 2d^4}{(a^2+2d^2)^{7/2}} \cdot \exp\left(-\frac{\xi^2}{a^2+2d^2}\right). \tag{7}$$

From these equations it is evident, that when the molecule is far from the location of the potential ($\xi \gg d$), the dynamics of the center-of-mass and width become independent. Namely, the center-of-mass freely moves with a constant velocity ($\xi_{tt} = 0$), and the width remains fixed in equilibrium state $a = a_0$, or oscillates with a constant frequency ω_0, if perturbed. The frequency of small amplitude oscillations can be found by expanding Eq.(6) around the fixed point $a(t) = a_0 + a_1(t), \quad a_1 \ll a_0$. Then we get the equation $a_{1tt} + \omega_0^2 a_1 = 0$, where

$$\omega_0 = \left(\frac{3}{a_0^4} - \frac{qN}{2\sqrt{2\pi}a_0^3} - \frac{gN}{2\sqrt{2\pi}} \cdot \frac{a_0^4(2a_0^2-5w^2) + 4w^4(6a_0^2-w^2)}{(a_0^2+w^2)^{9/2}}\right)^{1/2}. \tag{8}$$

Decoupling of equations (6)-(7) occurs due to vanishing of the action of the potential at large distances ($\xi \gg d,\ a$), since $\exp[-\xi^2/(a^2+2d^2)] \to 0$, and as a consequence, $G(a,\xi) \to 0$.

In the following sections we shall consider the scattering of a soliton molecule by weak and strong potential barriers and wells. The sketch of numerical experiments is illustrated in Fig. 1. Comparing the predictions of the VA with the results of numerical simulations of the GPE (1) will show the accuracy of the developed mathematical model.

3. Weak potential barriers and wells

The external potential is considered to be weak if its strength V_0 is much less than the amplitude of individual solitons A_s, forming the molecule. The maxima of the molecule's waveform (4) are located at $x = \pm a$, which can be found from the condition $d|\psi|/dx = 0$ at $\xi = 0$. Then the amplitude of individual soliton is

$$A_s = Aae^{-1/2} = \sqrt{\frac{2N}{ae\sqrt{\pi}}}. \tag{9}$$

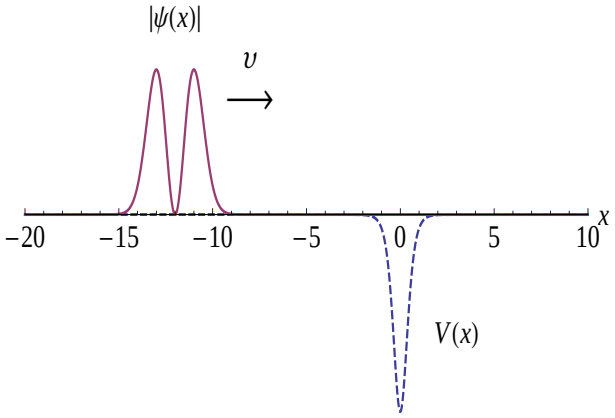

Figure 1. The sketch of numerical experiments. A two-soliton molecule is set in motion towards the external potential $V(x)$ with some initial velocity v. Depending on the strength of the potential and initial velocity, the molecule can be reflected, trapped or transmitted through the potential. If the potential is sufficiently strong and the velocity is high, the molecule can break up into individual solitons after the scattering event.

For instance, the amplitude of solitons, forming the molecule with norm $N = 2$ and parameter value $a = 1.87$, is equal to $A_s = 0.67$. These values are found from the fixed point ($a_{tt} = 0$) of Eq. (6) at $V_0 = 0,\ w = 5$, for pure dipolar condensate ($q = 0,\ g = 20$). Then the external potential with strength $|V_0| \ll A_s$ will be considered as a weak potential.

In Fig. 2 we illustrate the scattering of a two soliton molecule by weak potential barrier located at the origin ($x = 0$). At low velocity the molecule exhibits full reflection, while at greater velocity it is transmitted through the potential. As can be seen from Fig. 2b, after the interaction with the potential barrier the periodic exchange of matter between solitons takes place, which is caused by the collision induced pase shift. Deviation of the relative phase between solitons from π is responsible for the exchange of matter between them [11]. This is not accounted by the trial function (4), and therefore matter exchange cannot be described by the developed VA. Comparison with predictions of VA shows, that scattering by weak potential slightly perturbs the molecule, by exciting its internal modes. The agreement between VA and GPE is quite well for the center-of-mass dynamics, while for the width the agreement is only qualitative. These parameters are retrieved from the results of GPE simulation $\psi(x,t)$ as follows

$$\xi(t) = \frac{1}{N}\int_{-\infty}^{\infty} x\,|\psi(x,t)|^2 dx, \qquad a(t) = \left(\frac{2}{3N}\int_{-\infty}^{\infty}(x-\xi(t))^2\,|\psi(x,t)|^2 dx\right)^{1/2}. \tag{10}$$

It should be noted, that small amplitude oscillations of the width in GPE simulations before the scattering event is due to the approximate waveform of the molecule, obtained from VA. When the numerically exact waveform for the molecule is employed [11], these oscillations do not show up.

Extensive numerical experiments have shown that, scattering on weak potential barriers and wells mainly result in perturbation of the molecule, by exciting its internal modes and inducing the matter exchange between solitons. The same pertains to smooth potential barriers and wells, when the variation of the potential on the spatial scale of the molecule is small. In these limits the VA gives reliable predictions for the dynamics of soliton molecules. In particular, the period

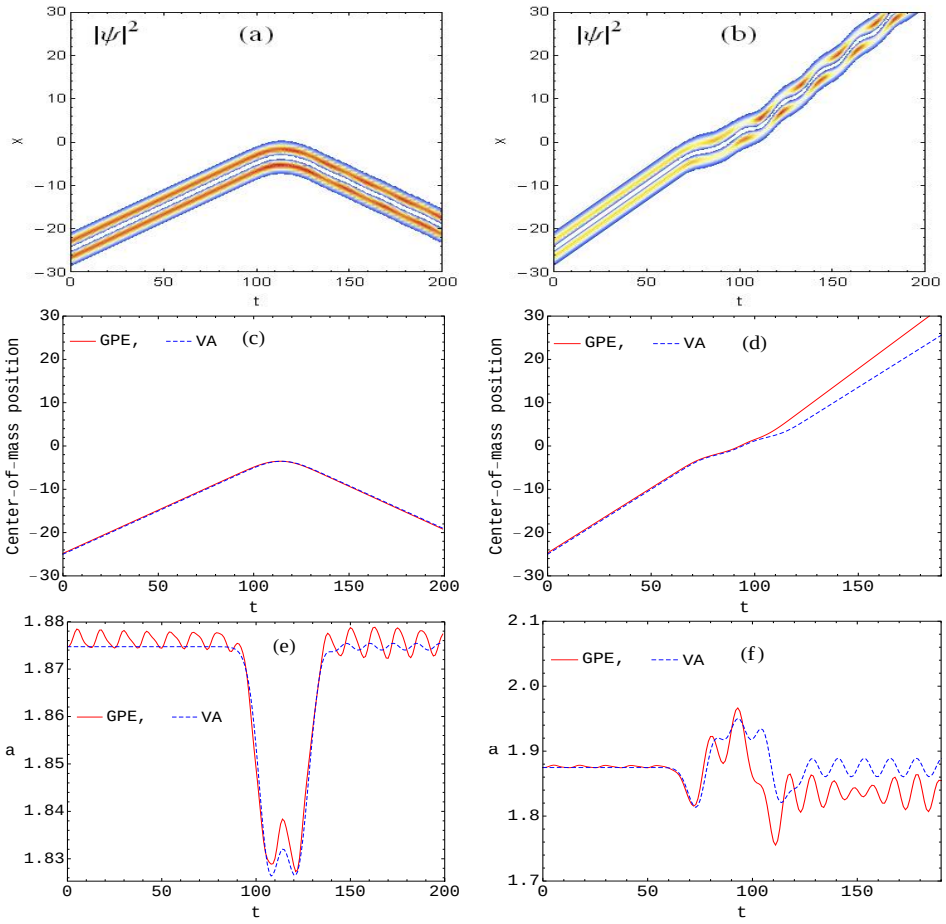

Figure 2. Scattering of a two-soliton molecule by weak potential barrier with $V_0 = 0.1$ at different velocities. Full reflection at low velocity $v = 0.2$ (a) and transmission at greater velocity $v = 0.3$ (b), according to GPE (1). Comparison GPE vs. VA for the center-of-mass position (c,d). At low velocity the two curves overlap (c), while at greater velocity there is a notable deviation after the scattering event (d). Agreement is only qualitative for the width (e,f). Initial parameter values $A = 0.585$, $a = 1.875$ are predicted by VA for $q = 0$, $g = 20$, $w = 5$, $N = 2$, $\xi_0 = -25$, $d = 1$.

of small amplitude oscillations of the width, shown in Fig. 2 (e) and (f), is very close to the VA predicted value in Eq. (8) $T = 2\pi/\omega_0 \simeq 12$.

4. Strong potential barriers and wells

In accordance with the definition, given in the previous section, by strong potential barriers and wells we presume the settings, when the strength of the potential is comparable or greater than the amplitude of individual solitons $|V_0| \gtrsim A_s$. In addition, the spatial extent of the potential is commensurate with that of the molecule $d \sim a$.

At low velocity of the soliton molecule, incident upon the strong potential barrier, the character of scattering is similar to the case of weak potential considered in the previous section. Namely, the molecule preserves its integrity after the reflection from the potential, while oscillations of solitons near their equilibrium position is excited, and matter exchange between them is induced. The dynamics of the center-of-mass and width still can be described by VA on a qualitative level. In the case of a potential well and sufficiently low velocity of the

molecule, the phenomenon of quantum reflection can be observed, which will be considered in the next section. Below we study scattering of a soliton molecule by strong potential barriers and wells, at moderately large velocities. Since the molecule undergoes significant deformation during the interaction process, and can be eventually disintegrated, the agreement between GPE and VA is not expected in these conditions. Therefore, our studies in this section will be mainly based on numerical experiments.

In Fig. 3 we illustrate the main characteristic features of scattering of a two-soliton molecule by Gaussian potential wells and barriers.

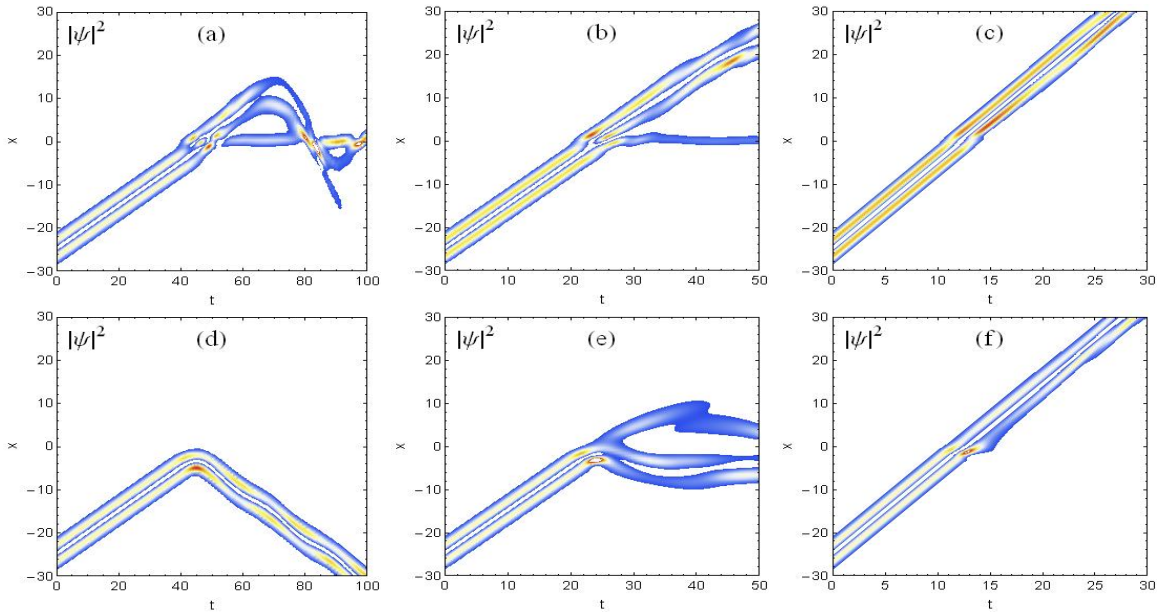

Figure 3. Scattering of a two-soliton molecule by strong potential well $V_0 = -1$ (upper row) and barrier $V_0 = 1$ (lower row) at different velocities, according to GPE (1). The molecule is destroyed by the potential well at moderately low velocity $v = 0.5$, comparable with $v_c = a_0\omega_0/\pi \simeq 0.3$ (a). At greater velocity $v = 1$ partial trapping of matter by the potential well occurs, and the remaining part traverses the well keeping its molecular structure (b). At even greater velocity $v = 2$ the molecule preserves its shape and almost intact transmission occurs (c). Low velocity collision at $v = 0.5$ with a strong potential barrier slightly perturbs the molecule (d). At greater velocity $v = 1$ the molecule is destroyed (e). At $v = 2$ the molecule can pass the barrier preserving its shape (f). Initial parameter values are similar to previous figure.

The length scales, associated with the soliton molecule and external potential are equal to $l_s = 2a$ and $l_p = d$, respectively. The greater of these two parameters defines the interaction time of the soliton molecule with the potential. In numerical simulations we use the narrow potential ($l_p < l_s$). The result of scattering depends on the ratio between the interaction time of the soliton molecule with a narrow potential $t_{int} \sim 2a_0/v$ and nonlinear relaxation time $T = 2\pi/\omega_0$. The characteristic velocity follows from the relation $t_{int} \sim T$, and is given by $v_c = a_0\omega_0/\pi$. When collision occurs at a velocity range, exceeding the quantum reflection threshold, but comparable with v_c, the molecule is destroyed by the potential well, as shown in Fig. 3a. In both cases of potential wells and barriers, collisions at high velocity ensure short interaction time, and soliton molecule can retain its coherence after the scattering event, as shown in Fig. 3 (c) and (f).

5. Quantum reflection of soliton molecules

A counterintuitive phenomenon of quantum reflection of matter-wave solitons from attractive potential wells was reported for the first time in [1]. Later the phenomenon was investigated in more details, theoretically [17] and experimentally [4]. The effect of accelerated motion of matter-wave solitons and two-soliton compounds, traversing the potential well, alongside with the quantum reflection phenomenon, was studied in [3]. Below we consider the effect of quantum reflection for two-soliton molecules.

The setting for numerical simulation of the quantum reflection is illustrated in Fig. 1. For the attractive potential well we consider the reflectionless Pöschl-Teller potential

$$V(x) = V_0 \,\mathrm{Sech}^2(\alpha x), \quad V_0 < 0. \tag{11}$$

The molecule with initial position x_0 is set in motion with velocity v towards the potential well (11). We assume that the process of interaction starts at time $t_0 \simeq x_0/v$, and finishes at $t_1 \simeq 2t_0$. Then the coefficients of reflection, transmission and trapping are calculated as follows

$$R = \frac{1}{N}\int_{-\infty}^{-h} |\psi(x,t_1)|^2 dx, \qquad T = \frac{1}{N}\int_{h}^{\infty} |\psi(x,t_1)|^2 dx, \qquad L = \frac{1}{N}\int_{-h}^{h} |\psi(x,t_1)|^2 dx, \tag{12}$$

where h denotes the position on the x-axis, at which the effect of the potential vanishes $V(h) \sim 0$, and N is the 1D norm of the soliton molecule.

The results of numerical simulations are presented in Fig. 4. For specified parameters the

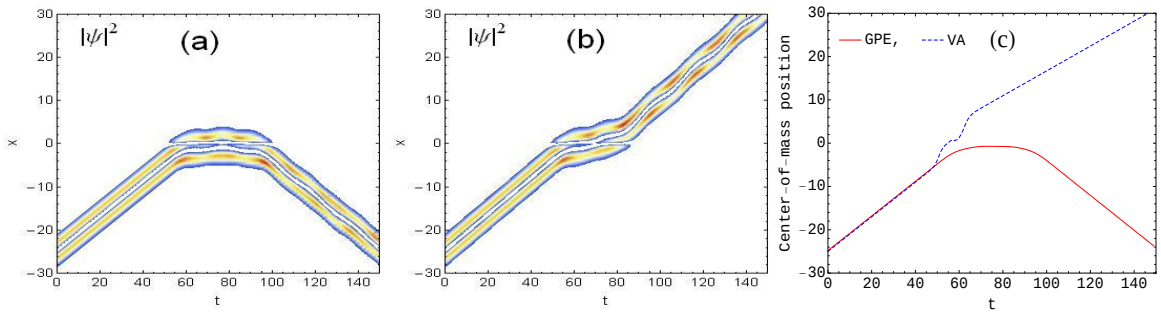

Figure 4. Quantum reflection at under-critical velocity $v = 0.40$ (a) and transmission at over-critical velocity $v = 0.42$ (b) of a two-soliton molecule, incident on the Pöschl-Teller potential well $V(x) = V_0 \,\mathrm{Sech}^2(\alpha x)$ with $V_0 = -4$ and $\alpha = 2$, according to GPE (1). Quantum reflection on panel (a) cannot be described by VA with a trial function (4), which is evident from the discrepancy after the scattering event (c).

quantum reflection of a two-soliton molecule from attractive potential takes place at velocities, below the critical value $v_q = 0.41$. At slower collision with $v = 0.40 < v_q$ we observe the full reflection ($R \simeq 1, \quad T \simeq 0$), while at slightly greater velocity $v = 0.42 > v_q$ the full transmission ($R \simeq 0, \quad T \simeq 1$) occurs. The physical mechanism behind the phenomenon of quantum reflection is linked to population of quantum states in the potential well by approaching soliton [1], as clearly observed in Fig. 4a. If the emerging localized state in the potential well has anti-phase configuration with respect to approaching soliton, they repel each-other, which results in reflection of the soliton.

Since the VA with a trial function (4) leads to equation of motion for the molecule's center-of-mass position, which is similar to equation for a particle in some external potential, it cannot describe the quantum reflection, as indicated by discrepancy after the scattering event, shown in

Fig. 4c. Incorporation of the quantum reflection into the frame of VA is possible by taking into regard the immobile trapped mode in the potential well [1, 18]. In all numerical experiments and calculations according to Eq. (12), the radiative and trapped parts of the field were negligible ($L \simeq 0$). This is the manifestation of the reflectionless property of the Pöschl-Teller potential, held in the nonlinear regime.

It should be pointed out, that the reflection from the potential well, shown in Fig. 4a would not be possible if the soliton molecule was ordinary particle, because there is no classical turning point for it in this potential. Therefore, the quantum reflection in the present context is understood as a classically forbidden reflection.

6. Conclusions

The scattering of a two-soliton molecule by Gaussian potential barriers and wells, described by the nonlocal Gross-Pitaevskii equation, has been studied by variational approximation and numerical simulations. Interaction with weak potentials gives raise to excitation of internal modes of soliton molecules and leads to matter exchange between solitons. When the potential is strong and collision velocity is moderately high, the molecule can break up and partially trapped by the potential well. At sufficiently high collision velocity the molecule again preserves its coherence, because during short interaction period with the potential the nonlinear relaxation and rearrangement processes cannot fully develop. In numerical experiments we observed the quantum reflection of a two-soliton molecule from the Pöschl-Teller potential well and found the critical velocity, at which the full reflection changes to full transmission. Predictions of the developed model, based on the variational approach, corroborate with the results of numerical simulations of the governing equation. Advantages and limitations of the variational method, applied to soliton scattering problems are discussed.

7. Acknowledgements

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