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Scattering of matter waves in spatially inhomogeneous environments

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We study scattering of quasi-one-dimensional matter waves at an interface of two spatial domains, one with repulsive and one with attractive interatomic interactions. It is shown that the incidence of a Gaussian wave packet from the repulsive to the attractive region gives rise to generation of a soliton train. More specifically, the number of emergent solitons can be controlled, e.g., by the variation of the amplitude or the width of the incoming wave packet. Furthermore, we study the reflectivity of a soliton incident from the attractive region to the repulsive one. We find the reflection coefficient numerically and employ analytical methods, which treat the soliton as a particle (for moderate and large amplitudes) or a quasilinear wave packet (for small amplitudes), to determine the critical soliton momentum (as a function of the soliton amplitude) for which total reflection is observed.

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I. INTRODUCTION

For almost two decades, the study of nonlinear phenomena occurring in atomic Bose-Einstein condensates (BECs) has experienced an enormous increase of interest [1,2]. Prominent examples, in the quasi-one-dimensional (1D) setting, are the experimental observation of robust matter-wave solitons of the bright and dark type and the study of their nonlinearity, has also been extensively studied. In particular, inhomogeneous condensates [15] with a spatially modulated spatial domain, which gives rise to the so-called collisionally inhomogeneous nonlinear lattice) variations, can be found in Ref. [25]. It should be noted in passing that similar studies have also been performed in the context of nonlinear optics; relevant investigations include (but are not limited to) light-beam scattering at interfaces separating nonlinear dielectric media [26], transformation of waves passing an interface between regions of normal and anomalous group-velocity dispersion [27], and surface soliton dynamics at interfaces between inhomogeneous periodic media [28].

In this work, we study the scattering of matter waves in a collisionally inhomogeneous environment. In particular, we consider a quasi-1D setting (whereby matter waves are oriented along the x direction) and assume that the scattering length a is piecewise constant for x < 0 and x > 0, taking, respectively, the values \(-a_1 < 0\) and \(a_2 > 0\), and changes sign at x = 0. In other words, we assume that the normalized scattering length \(a(x)\) takes the form

\[
 a(x) = \frac{1}{2} \left[ \left( \frac{a_2}{a_1} - 1 \right) + \left( \frac{a_2}{a_1} + 1 \right) \tanh \left( \frac{x}{W} \right) \right],
\]

where W is the spatial scale over which the transition between the asymptotic values \(a_1\) and \(a_2\) takes place. For the above setting, in the framework of the mean-field approximation, we will investigate two different scattering processes; a description of our considerations and the organization of the paper are as follows.

First, in Sec. II, we study the incidence of a nearly linear (Gaussian) wave packet from the repulsive region (x > 0) to the attractive region (x < 0) and demonstrate the generation of a train of bright solitons. By numerically integrating the pertinent Gross-Pitaevskii (GP) equation, we determine the number of created solitons as a function of the initial
data (amplitude, width, and momentum of the incident wave packet), as well as the difference of the values of the scattering length.

In Sec. III, we study the reflectivity of a bright soliton from the scattering length interface; the soliton is assumed to exist and travel from the attractive region \((x < 0)\) towards the repulsive region \((x > 0)\). We find numerically the reflection coefficient as a function of the soliton momentum and amplitude and find that it has a steplike dependence on momentum for sufficiently weak solitons. In the case of total reflection, we use an analytical approximation (treating the soliton as a particle) and find the equation of motion for the soliton center. This equation is used to determine the critical value of momentum below which total reflection occurs, which turns out to depend linearly on the soliton amplitude. Additionally, for extremely weak solitons, employing results from linear quantum mechanics \([29]\), we also find a (different) linear dependence of the critical momentum on the soliton amplitude. Both analytical estimates for weak and strong solitons are found to be in very good agreement with the numerical results, with the latter also encompassing a transition region between the two regimes.

Finally, Sec. IV summarizes our findings and presents a number of directions for future study.

II. REFLECTIVITY OF A GAUSSIAN WAVE PACKET FROM THE SCATTERING LENGTH INTERFACE

Model and creation of a soliton train

Our considerations start from the following GP equation, which describes a quasi-1D BEC oriented along the \(x\) axis \([1,2]\):

\[
i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + 2\hbar\omega_\perp a |\Psi|^2 \Psi. \tag{2}
\]

Here \(\Psi(x,t)\) is the mean-field order parameter, \(m\) is the atomic mass, \(\omega_\perp\) is the transverse confining frequency, and \(a\) the \(s\)-wave scattering length \([a > 0 \quad (a < 0)]\) corresponds to repulsive (attractive) interatomic interactions. Considering a situation where proper spatially dependent fields close to Feshbach resonances are employed, we assume that the scattering length \(a\) is piecewise constant for \(x < 0\) and \(x > 0\), taking the form

\[
a(x) = (1/2)[(a_2 - a_1) + (a_1 + a_2) \tanh(x/W)], \tag{3}
\]

where \(W\) is the spatial scale over which the transition from the asymptotic value \(a_1, a_2 < 0\) (for \(x/W \to -\infty\)) to \(a_2 > 0\) (for \(x/W \to +\infty\)) takes place.

A strategy for developing a corresponding experimental implementation can be based on the interaction tunability of specific atomic species by applying external magnetic fields. For example, for cesium the \(s\)-wave scattering length \(a\) changes sign through a zero crossing at an external field strength of 17 G \([30]\). Confining cesium atoms in an elongated trapping potential near the surface of an atom chip \([31]\) will allow for appropriate local engineering of \(a\) to form steps of varying widths \(W\), where the atom-surface separation sets a scale for achievable minimum step widths. The trapping potential can be formed optically, possibly also by a suitable combination of optical and magnetic fields, whereby care has to be taken as the magnetic field will influence both the external potential and the scattering length profile \(a(x)\); see e.g. the relevant discussion of \([32]\).

Normalizing time and space in Eq. (2), as \(t \to \omega_\perp t\) and \(x \to x/a_\perp\) [where \(a_\perp = (\hbar/\omega_\perp)^{1/2}\) is the transverse harmonic oscillator length] and the density as \(|\Psi|^2 \to 2a_\perp |u|^2\), we cast Eq. (2) into the following dimensionless form:

\[
\frac{i}{\hbar} \frac{\partial u}{\partial t} + \frac{1}{2} \frac{\partial^2 u}{\partial x^2} - a(x) |u|^2 u = 0, \tag{4}
\]

where the function \(a(x)\) is given by Eq. (1). For our analytical and numerical considerations below, we will use the values \(a_2/a_1 = 0.95\) and \(W = 0.01\). The former choice is made so as to consider the case in which \(a_1\) and \(a_2\) take similar values (and not, e.g., cases with \(a_2/a_1 \ll 1\) or \(a_2/a_1 \gg 1\); the specific value \(a_2/a_1 = 0.95\) is not crucial for our analysis, i.e., qualitatively similar results are obtained for other similar choices. On the other hand, the choice \(W = 0.01\) corresponds to an abrupt steplike transition from the repulsive to the attractive region.

It is relevant to point out here that, generally, Eq. (2) and its variants attempting to more adequately capture transverse degrees of freedom (see the quasi-1D models of Refs. \([33,34]\)) suggest that the variations or modulations in transverse trapping strength can be used in a way equivalent to longitudinal variations of the scattering length. This idea has been used even in a quantitative fashion, e.g., to explain the phenomenology of the formation of Faraday wave patterns (see Refs. \([23,35]\)). Nevertheless, this type of consideration is not applicable in the present setting, given the sign-changing nature of the nonlinearity.

We now assume that a Gaussian wave packet of amplitude \(U_0\) and width \(l\), initially located at \(x = x_0 > 0\) (i.e., in the repulsive region), moves towards the attractive region. The specific form of the wave packet, which is used as an initial condition for Eq. (4) in our simulations, is

\[
u(x,0) = U_0 \exp\left(-\frac{(x-x_0)^2}{l^2}\right) \exp(-iKx), \tag{5}
\]

where \(K\) is the initial momentum of the wave packet. Notice that this form of the wave packet approximates the ground-state profile that would be created in (and potentially released from, in an experimentally relevant setting) a parabolic trap in the repulsive region under consideration and in the case of relatively small atom numbers (corresponding to a weak nonlinearity).

Using the parameter values \(x_0 = 20, l = 10,\) and \(K = 1.5\) (as well as \(U_0 = 1, W = 0.01,\) and \(a_2/a_1 = 0.95\)), we depict the corresponding configuration in the top panel of Fig. 1. In the middle and bottom panels of the same figure, we show the subsequent dynamics: It can be observed that the wave packet is transmitted through the discontinuity of the scattering length at \(x \approx 0\) and, after entering the region with attractive interactions, transforms into a train of bright solitons; for a recent discussion of these non-dispersive wave packets and their interactions, including an experimental exploration of their collisions, see e.g. Ref. \([36]\). Notice that the soliton-generation process is such that each generated soliton is larger than the one that will be generated at a later time. This is due to the fact that once a portion of the condensate enters the
profiles of the wave function at interactions. The top and middle panels show, respectively, the density in the region with repulsive interactions to the region with attractive interactions. The bottom panel shows the normalized scattering length profile for $a$, and characteristics of the atomic soliton train described above. The top and middle panels show, respectively, the density of the produced solitons' velocities. A velocity equal to its initial one, which is generally different from the repulsive region) spreads as it approaches the step, having an initial Gaussian wave packet (which is not an exact solution in solitons is the same. Additionally, it should be noted that the number of the created solitons is 7 at time $t=200$. Here we should note that for the counting of the number of solitons, we have included only solitons of amplitude of at least 10% of the first created soliton.

III. REFLECTIVITY OF A SOLITON FROM THE SCATTERING LENGTH INTERFACE

Next we consider the reflectivity of a bright soliton at the scattering length interface. We assume in particular that a bright soliton moves from the attractive ($x<0$) to the repulsive region ($x>0$) and is thus scattered at the interface, at $x=0$, caused by the change of the sign of the nonlinearity. This dynamical scenario is effectively complementary to the one studied in Sec. II.

The bright soliton propagating in the attractive region has the form

$$u(x,t) = \eta \sech[\eta(x - x_0(t))] \exp[i(kx - \omega t)],$$

where $\eta$, $k$, $x_0$, and $\omega$ respectively denote the amplitude, velocity, initial position, and frequency of the soliton. Then we numerically integrate Eq. (2) with the initial condition of a somewhat different physical mechanism: In that work, the soliton train was produced via a sufficiently deep spatially dependent nonlinearity that acted on a trapped Gaussian wave packet (existing between regions of vanishing and negative scattering lengths). The depth of the (abrupt) negative step was found to control the number of emitted solitary waves. We find that number of the created solitons $N_s$ depends on the momentum $K$, the amplitude $U_0$, and the width $l$ of the Gaussian wave packet, as well as the height of the interface $a_2/a_1$. Results pertaining to the count of the soliton number are shown in Fig. 2: Larger initial amplitudes and/or widths of the wave packet result in a larger number of solitons. On the other hand, increasing the initial momentum $K$ and/or the height $a_2/a_1$ of the interface seems to have a weaker effect on the process; for the particular example shown in Fig. 1, the number of solitons is 7 at time $t=200$. Here we should note that for the counting of the number of solitons, we have included only solitons of amplitude of at least 10% of the first created soliton.
FIG. 3. (Color online) Contour plots showing the evolution of the density of a bright soliton of initial velocity \( k = 0.7 \), scattered at the interface between the attractive and repulsive regions, at \( x = 0 \) [depicted by the dashed (white) line]. From top to bottom, the amplitude of the soliton is \( \eta = 0.2, 0.6, \) and 1. The top (bottom) panel corresponds to total transmission (reflection); the middle panel shows partial reflection.

The soliton reflectivity can be calculated numerically upon determining the reflection coefficient \( R \), defined as the number of atoms remaining in the \( x < 0 \) (attractive) region over the number of atoms of the incident soliton. Taking into consideration that the latter is given by \( \int_{-\infty}^{0} |u(x,0)|^2 dx = 2\eta \), we can express \( R \) as

\[
R = \frac{1}{2\eta} \int_{-\infty}^{0} |u(x,t^*)|^2 dx. \tag{8}
\]

Here \( t^* \) is a time sufficiently large such that the reflected and transmitted parts of the soliton are spatially well separated; this separation is set by a spatial region of extent \( \Delta x \approx k_t^* \) around \( x = 0 \) and, accordingly, \( t^* \) is appropriately chosen for each individual numerical experiment.

Figure 4 shows the reflection coefficient as a function of the initial soliton momentum \( k \), for various values of large soliton amplitudes \( \eta \). The inset shows cases corresponding to weak solitons.

FIG. 4. (Color online) Reflection coefficient \( R \) as a function of the initial soliton momentum \( k \), for various values of large soliton amplitudes \( \eta \). The inset shows cases corresponding to weak solitons.

\[ R = \frac{1}{2} \int_{-\infty}^{\infty} \frac{\partial u(x,0)}{\partial x} \frac{\partial u(x,t)}{\partial x} dx, \tag{9} \]

which is connected with the soliton momentum \( P = (i/2) \int_{-\infty}^{\infty} (u^* x - u^* u_x) dx \). Then, differentiating the latter expression with respect to \( t \) and using Eq. (4), it is straightforward to derive the following equation of motion for \( \tau \):

\[
\frac{d^2 \tau}{dt^2} = \frac{1}{2} \int_{-\infty}^{\infty} \frac{\partial a(x)}{\partial x} (u(x,t))^4 dx. \tag{10} \]

The integral on the right-hand side of Eq. (10) can be calculated in an analytical form, upon approximating \( a(x) \) [see Eq. (1)] by a Heaviside function in the limiting case where \( W \ll 1/\eta \). Then \( da(x)/dx \) is approximated by a \$\delta \$ function and integrating the right-hand side of Eq. (10), we end up with the following result:

\[
\frac{d^2 x_0}{dt^2} \approx - \frac{1}{2} \left( 1 + \frac{a_2}{a_1} \right) \eta^4 \text{sech}^4 [\eta x_0(t)]. \tag{11} \]

Then, taking into consideration that the soliton center is connected with the center of mass through the equation \( \tau = 2\eta x_0 \), we can express Eq. (11) as follows:

\[
\frac{d^2 x_0}{dt^2} = - \frac{dV_{\text{eff}}}{dx_0}, \tag{12} \]

where the effective potential \( V_{\text{eff}} \) is given by

\[
V_{\text{eff}}(x_0) = \frac{1}{12} \left( 1 + \frac{a_2}{a_1} \right) \eta^4 [3 \tanh(\eta x_0) - \tanh^3(\eta x_0)]. \tag{13} \]
Equation (12) shows that the soliton can be regarded as a Newtonian unit-mass particle, which evolves in the presence of the effective potential $V_{\text{eff}}$; the latter has a shape of a steplike barrier, as depicted in Fig. 5. Thus, according to this particle picture, the soliton will be totally reflected if its initial energy $E_i$ is less than the height of the barrier. Since the soliton is expected to interact with the effective potential only through its exponential leading tail, the soliton center is anticipated to never reach the interface at $x = 0$, but it will approach it only up to a distance roughly equal to the half width at half maximum (HWHM) of the soliton; the above situation is schematically illustrated in Fig. 5. Thus, taking into consideration that the soliton’s HWHM, denoted by $\Delta x$, is connected with the inverse width $\eta$ through the equation $\Delta x = \ln(1 + \sqrt{2})/\eta$, we can find that the relevant barrier height is given by $V_{\text{eff}}(\Delta x) - V_{\text{eff}}(x_0(0))$, where $x_0(0)$ is the initial soliton position. According to the above arguments, the soliton will be totally reflected if the initial soliton energy is less than or equal to the effective barrier height, namely,

$$E_i \equiv \frac{1}{2} k^2 + V_{\text{eff}}(x_0(0)) \leq V_{\text{eff}}(\Delta x). \quad (14)$$

We have numerically checked the validity of this analysis by comparing first the numerically obtained soliton trajectory [by means of direct numerical integration of Eq. (4) in the case of total reflection] with the approximate analytical result of Eq. (12). A typical example, corresponding to a soliton amplitude $\eta = 0.4$ and momentum $k = 0.1$, is shown in Fig. 6. There the numerical result is displayed in the form of a contour plot for the evolution of the soliton density and the analytical result of Eq. (12) (see the dashed line in the figure). Note that similar results were obtained for soliton amplitudes $0.2 < \eta < 2$. It can be seen that the dashed line follows with fairly good accuracy the evolution of the soliton center. The slight discrepancy observed can be explained as follows: The tail of the bright soliton, in the case of total reflection (see Figs. 5 and 6), interacts with the interface, enters the repulsive area, and eventually returns to the attractive region. This effect, which cannot be explained via the particle approach, causes a slight shift in the soliton trajectory. Thus, the trajectory obtained from Eq. (10) has naturally a slight discrepancy for any soliton amplitude $\eta$.

Next, employing Eq. (14), it is possible to derive analytically the critical value of the initial momentum $k_{cr}$ [when the equality in Eq. (14) holds], for which total reflection occurs, as a function of the soliton amplitude and the parameters characterizing the scattering length profile. The result is

$$k_{cr} = \left[\frac{1}{3} \left(1 + \frac{a_2}{a_1}\right)(1 + C)^{-1/4}\right]/\eta, \quad (15)$$

where constant $C = (1/2)[3 \tanh(\eta \Delta x) - \tanh^3(\eta \Delta x)]$ and $\eta \Delta x = -\ln(1 + \sqrt{2}) \approx -0.88$. Note that Eq. (15) suggests a linear dependence of $k_{cr}$ on $\eta$, which is confirmed by our numerical simulations. Indeed, as shown in Fig. 7, for solitons of sufficiently large amplitudes, i.e., for $\eta \gtrsim 0.2$, this analytical prediction [depicted by the solid (green) straight line] is in excellent agreement with the numerical result for $k_{cr}$ [depicted by the (red) dots]. Notice that the numerically obtained values for $k_{cr}$ are calculated so that the respective reflection coefficient values become less than unity by a factor of $10^{-3}$; however, we note here that the results presented are only weakly sensitive to the selection of the particular threshold.
The reflection coefficient was determined numerically as a function of the initial soliton momentum for different soliton amplitudes. For sufficiently weak solitons, we found an almost abrupt change from total transmission to total reflection, effectively associated with the linear phenomenology in a step potential. For stronger solitons, the reflection coefficient featured a smoother dependence on the momentum.

We also developed analytical approximations, which treated the solitons as particles (for large amplitudes) or linear wave packets (for small amplitudes), to determine the critical value of soliton momentum $k_{cr}$ below which total reflection occurs. We found that $k_{cr}$ depends linearly on the soliton amplitude, but with different slopes in the purely nonlinear and the quasilinear regimes. Numerically, we found a smooth crossover between these two regimes, which can be interpreted as a gradual continuous change of the soliton from being dominated by wave-like to particle-like properties. Our analytical predictions were found to be in very good agreement with the corresponding numerical results.

There are numerous directions that may be worth investigating for future efforts. One of these is to consider the possibility of multiple steps and their interplay. Another is to examine the interplay of the nonlinear step with an external linear potential or with a nontrivial background (e.g., on the repulsively interacting side, which can support such a background) and to explore the dynamics of incident wave packets in such settings. Potentially, probing the soliton dynamics in such configurations could be utilized towards retrieving quantitative information about the nature of linear and/or nonlinear unknown potentials.

From a more rigorous mathematical perspective, it would be interesting to attempt to connect the present setting to the extensive developments in treating integrable problems with suitable boundary conditions (e.g., on the half line), as detailed, e.g., in Ref. [38]. A way to make this connection may be to consider the GP equation, e.g., solely on the attractive domain with a boundary condition inferred by the incidence of the Gaussian wave packet at $x = 0$ (i.e., a Gaussian in time boundary condition). A potential by-product of such a formulation might be the identification of the number of solitary waves that will emerge as a function of the properties of this effective (and localized in time) boundary drive.

Finally, it would be of particular interest to extend considerations to the two- or higher-dimensional setting. There, understanding the properties of the formed solitons, e.g., on the attractive interaction domain, taking into consideration the collapse feature that arises in the critical or supercritical higher-dimensional case [39], would be especially relevant.
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