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Reflection and transmission of matter waves in two-component Bose-Einstein condensates

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Reflection and transmission of matter waves in two-component Bose-Einstein condensates

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Abstract. We investigate the dynamical properties of 1D solitary waves in confined immiscible mixtures of Bose-Einstein condensates with repulsive interparticle interactions. We perform numerical simulations of the coupled Gross-Pitaevskii equations for two-components harmonically trapped in presence of dark and grey solitons, and we study the reflection and transmission of this matter wave after the collision with the interphase between the two immiscible species. Our numerical results show different scenarios depending on the ratio between the interspecies and intraspecies strength interactions, where the immiscibility plays an important role in the dynamical behaviour of the matter wave.

Keywords: Bose-Einstein condensates, two-component, matter wave, dark soliton, immiscibility

1. Introduction

In the last two decades, the phenomenon of Bose-Einstein condensation has become an increasingly active area of research, both experimentally and theoretically. A Bose-Einstein condensate (BEC) is a state of matter that a bosonic system reaches below a certain critical temperature. When the thermal de Broglie wavelength becomes comparable to the mean interparticle separation the transition to this state occurs. When this condition is attained, a macroscopic fraction of the bosons occupies the lowest single-particle quantum state. Bose-Einstein condensation plays remarkable roles in atomic, elementary particle, nuclear, condensed matter physics and astrophysics [1].

The prototype of a system of bosons undergoing Bose-Einstein condensation is the superfluid ^{4}He, but due to the strong interaction between helium atoms the condensate fraction, i.e. the ratio N_0/N between the number of condensed particles N_0 and the total number of particles N, is dramatically reduced. For this reason it is advisable to look for weakly interacting systems like ultracold atomic gases. Currently available systems that fulfill this condition are Bose-Einstein condensates of ultracold gases. The first BECs

of alkali atoms were realized in 1995 by using powerful laser-cooling methods [2, 3], providing unique opportunities for exploring quantum phenomena on a macroscopic scale. Due to the fact that in a BEC most of the atoms occupy the same quantum state, the condensate can be very well described in terms of a mean-field theory if the number of atoms is large enough. This is the so-called Gross-Pitaevskii (GP) theory, which has reproduced with excellent agreement different experimental results [4, 5], e.g. energy spectrum, quantized vortices, the superfluid response of the system against rotation, or the generation and motion of topological defects as solitons.

The amazing development in trapping techniques for BECs has allowed experimentalists to simultaneously confine atomic clouds in different hyperfine spin states or different atomic species. The first experiment involving interaction between multiple-species BECs was performed in rubidium atoms which demonstrated the possibility of producing long-lived multicomponent condensate systems [6]. A mixture of BECs can be produced experimentally by simultaneously trapping atoms in different hyperfine states or two isotopes of the same element or of different species. These multicomponent condensates can present new dynamics and scenarios due to the intercomponent interactions.

In this work we analyze the dynamical features of solitonic waves (solitons), which are analytical solutions of the one dimensional GP equation and have the peculiarity that they maintain their shape while propagate, in harmonically trapped one dimensional two-component BECs with repulsive interatomic interactions. We start by characterizing the solitons in homogeneous systems, in single-component BECs. Then, we perform numerical simulations to investigate the dynamical behaviour of dark solitons in two-component trapped condensates, in the immiscible case, where the repulsion between the species favours their spatial separation. Additionally, taking advantage of the oscillatory motion of dark solitons in harmonic traps we study the behaviour of this matter wave in the interphase between both species, defining a transmission and reflection coefficients from the conserved energy of the system.

2. Theory

The Gross-Pitaevskii theory is a mean-field approximation that provides a nonlinear Schrödinger equation for the wave function $\psi(\vec{r}, t)$ (also called the order parameter) that describes the condensate. It is valid when the system is dilute and weakly interacting, that is, when the s-wave scattering length a_s is much smaller than the average distance between atoms and the number of atoms in the dilute system becomes large enough [4]. The time-dependent GP equation is [4, 5]

$$i\hbar \frac{\partial}{\partial t} \psi = \left(-\frac{\hbar^2}{2m} \nabla^2 + V_{ext}(\vec{r}) + g|\psi|^2 \right) \psi , \qquad (1)$$

where $g = 4\pi\hbar^2 a_s/m$ is the interaction strength, m is the mass of the particles, $V_{ext}(\vec{r})$ is an external confining potential (needed to trap the particles), and ψ is normalized to the total number of particles $\int d\vec{r} |\psi|^2 = N$.

For stationary solutions $\psi(\vec{r}, t) = \psi(\vec{r}) \exp(-i\mu t/\hbar)$, where μ is the chemical potential, and the GP equation (1) becomes

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{ext}(\vec{r}) + g|\psi|^2\right)\psi = \mu\psi \ . \tag{2}$$

In the absence of interactions ($g = 0$) this equation reduces to the usual Schrödinger equation for the non-interacting hamiltonian. However, is precisely the effect of the interactions that yields the non-linear term in equation (2) and leads to interesting features such as solitonic solutions.

Exact solutions: dark solitons

In the one dimensional (1D) homogeneous case, $V_{ext} = 0$, the GP equation (2) admits analytical solutions. One particular kind of these solutions are the so-called solitons [4]. A soliton is a solitary matter wave that propagates preserving its intrinsic shape, and can interact with other solitons emerging unchanged from the collision, except for a phase shift [7]. There are mainly two different solitonic solutions depending on the sign of the interaction: the bright and the dark (grey) soliton for attractive and repulsive interactions, respectively. Both solutions correspond to a localized modulation of the density profile characterized by an increase (bright) or a depletion (dark, or grey if the suppression is not total) of the density with respect to the homogeneous value. The typical length characterizing the extension of the density modulation is fixed by the healing length ξ.

If the interaction is attractive ($g < 0$), the stationary solitonic solution corresponds to a bright soliton with functional form $\psi(x) \propto \mathrm{sech}(x/\sqrt{2}\xi)$ and negative chemical potential. This type of solitons can move freely in space (along the x-direction) like an ordinary particle. Although bright solitons are not stable configurations in higher dimensional systems, they can be produced in traps with tight radial confinement, where the mechanism of destabilization is reduced [8].

In this work we focus on the case of repulsive interparticle interactions ($g > 0$), where there exists an analytical solution of an excited state of the GP equation (1) that corresponds to a solitary matter wave moving with constant velocity v on a constant background [9]:

$$\psi_s(x, t) = \sqrt{n}\left(i\frac{v}{c} + \sqrt{1 - \left(\frac{v}{c}\right)^2}\tanh\left[\frac{x - vt}{\sqrt{2}\xi}\sqrt{1 - \left(\frac{v}{c}\right)^2}\right]\right), \tag{3}$$

where n is the background (ground state) constant density, $c = \sqrt{gn/m}$ is the speed of sound and the healing length is given by $\xi = \hbar/\sqrt{2mgn}$. The density profile $n(x) = |\psi_s|^2$ has a minimum at the center of the soliton corresponding to $n(0) = nv^2/c^2$. Notice that for the static case ($v = 0$), i.e. the dark soliton, the minimum density is equal to zero. The width of the soliton is fixed by the healing length ξ and amplified by the factor
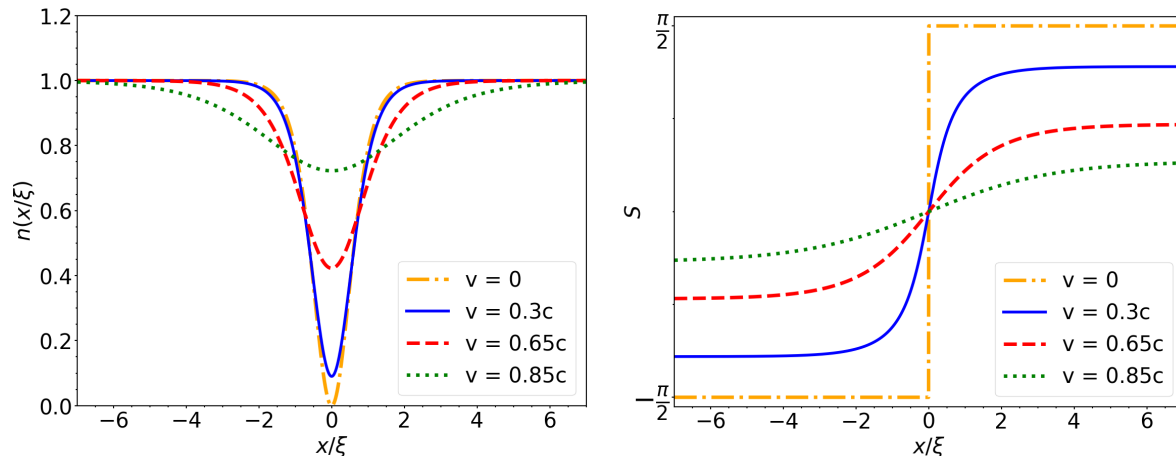
Figure 1. Density profile (left panel) and phase (right panel) of a 1D dark and moving grey soliton with different velocities in an homogeneous background with density $n = 1/\xi$.

$1/\sqrt{1 - (v/c)^2}$, which increases as v approaches c. The chemical potential is positive and is fixed by the background density where the condensate is living, $\mu = gn$.

In contrast to the bright soliton case, dark (and grey) solitons present topological features that deserve further analysis. Dark solitons can be seen as topological defects connecting two ground states with the same density but different phase [10]. The phase S of the wave function $\psi_s(x) = \sqrt{n(x)}e^{iS(x)}$ undergoes a finite change as x varies from $-\infty$ to $+\infty$:

$$\Delta S = S(\infty) - S(-\infty) = 2 \cos^{-1}\left(\frac{v}{c}\right) . \tag{4}$$

For a static dark soliton the phase change is given by $\Delta S = \pi$ and its wave function $\psi_s(x) = \sqrt{n} \tanh(x/\sqrt{2}\xi)$ becomes real.

Figure 1 shows the characteristic density profiles (left panel) and phases (right panel) of moving grey solitons with varying velocity. As can be seen, the width of the soliton, which is proportional to the healing length ξ, increases as v approaches c. On the other hand, the phase change ΔS increases up to π as v approaches zero.

The excitation energy ε_s of the soliton can be evaluated as the difference between the energies in presence and in absence of the soliton. It yields the following analytical expression [11]:

$$\varepsilon_s(\mu, v) = \frac{4}{3}\frac{\hbar m}{g}\left(\frac{\mu}{m} - v^2\right)^{3/2} . \tag{5}$$

It is worth noticing that the velocity of the soliton increases when its energy decreases. As $v \to c$ the excitation energy of the soliton tends to zero, and the nonlinear solitonic solution to the GP equation converges with the linear sound excitations (phonons) of the constant ground state.

The topological nature of dark solitons makes them dynamically stable states (i.e. stable in the absence of dissipation). However, in 2D and 3D systems, they are unstable

with respect to fluctuations along the transverse directions (y and z). This instability can be largely suppressed in experiments by squeezing the condensate in the transverse direction, as highly elongated cigar-shaped traps do [12].

Coupled Gross-Pitaevskii equation

We consider a mixture of two coupled BECs confined in the same external potential V_{ext}, described by the wavefunctions ψ_1 and ψ_2, and with N_1 and N_2 atoms, respectively. The system is described by two coupled GP equations in the mean-field regime [5]:

$$i\hbar\frac{\partial}{\partial t}\psi_1 = \left[-\frac{\hbar^2}{2m_1}\nabla^2 + V_{ext} + g_{11}N_1|\psi_1|^2 + g_{12}\sqrt{N_1 N_2}|\psi_2|^2\right]\psi_1 \ ,$$

$$i\hbar\frac{\partial}{\partial t}\psi_2 = \left[-\frac{\hbar^2}{2m_2}\nabla^2 + V_{ext} + g_{21}\sqrt{N_1 N_2}|\psi_1|^2 + g_{22}N_2|\psi_2|^2\right]\psi_2 \ , \qquad (6)$$

where $g_{ij} = 2\pi\hbar^2 a_{ij}/m_{ij}$ ($i,j = 1,2$) and $m_{ij} = m_i m_j/(m_i + m_j)$ is the reduced mass. The coupling constants g_{11}, g_{22}, $g_{12} = g_{21}$ are related to the intraspecies scattering lengths a_{11} and a_{22}, and to the interspecies scattering length $a_{12} = a_{21}$, respectively. The self-interaction is attractive in the case $a_{jj} < 0$ and repulsive for $a_{jj} > 0$, whereas the interspecies interaction is repulsive when $a_{12} > 0$ and attractive when $a_{12} < 0$. The wavefunctions are normalized to unity.

A key feature of mixtures is that they can exhibit miscibility or immiscibility behaviour depending on the strength of the interactions. Miscibility, when the interactions favour an overlap between the two species ($g_{11}\,g_{22} > g_{12}^2$), and immiscibility, when the repulsive interaction between the two species favours their spatial separation ($g_{11}\,g_{22} < g_{12}^2$) [13]. In this work we focus in the immiscibility behaviour.

3. Results and discussion: matter waves in two-component BECs

We want to study the behaviour and dynamics of dark solitons in two-component BECs in the immiscible regime. In particular, the reflection and transmission of a matter wave in one component when it collides with the interphase between the two species. In order to do so it is necessary to perform a real time evolution, since the soliton is under motion. With this aim is very important to choose properly the external potential. We have considered two types of confinement: harmonic and box potential. If we use box potentials the density is constant and the soliton remains static, thus a kick is needed in order to make it move. This kick may cause slight vibrations of the whole condensate which are not convenient for our work. In contrast, if we use harmonic potentials the soliton motion is oscillatory which will cause the soliton to move towards the interphase between the species as it is needed for this work. In what follows, we consider a mixture of two BECs confined by the same 1D harmonic potential. One dimensional harmonic potentials are experimentally accessible by using large harmonic

frequencies in the transverse y–z plane, focusing on elongated geometries of the system along the x-direction $V_{ext}(x, y, z) = \frac{1}{2} m(\omega_x x^2 + \omega_\perp(y^2 + z^2))$, assuming that $\omega_\perp \gg \omega_x$, so that the transverse degrees of freedom are frozen, and the system shows effective 1D dynamics along the x-direction. As a consequence, the interaction strengths entering the GP equation have to be renormalized as [4]

$$g_{ij} = \frac{\hbar^2}{m_{ij}} \frac{a_{ij}}{a_\perp^2} , \tag{7}$$

where $a_\perp$ is the characteristic length of the transverse harmonic oscillator. In our particular case, we have assumed that the mass of the atoms of both species is the same $(m_1 = m_2)$. This could be achieved, for instance, using the same atom for both species but in different hyperfine states.

We start by characterising the different coupled states of the immiscible mixture we are dealing with, namely solitonic and ground state in a 1D harmonic trap. To obtain these states we solve numerically the coupled GP equations (6) by using the Trotter-Suzuki Python package [14]. The heart of the Trotter-Suzuki Algorithm is the decomposition of the dynamics into sets of small unitary evolutions, allowing parallelization, which decreases the computational time of the numerical simulations. In the soliton case, our initial ansatz contains a node at an off-center location.
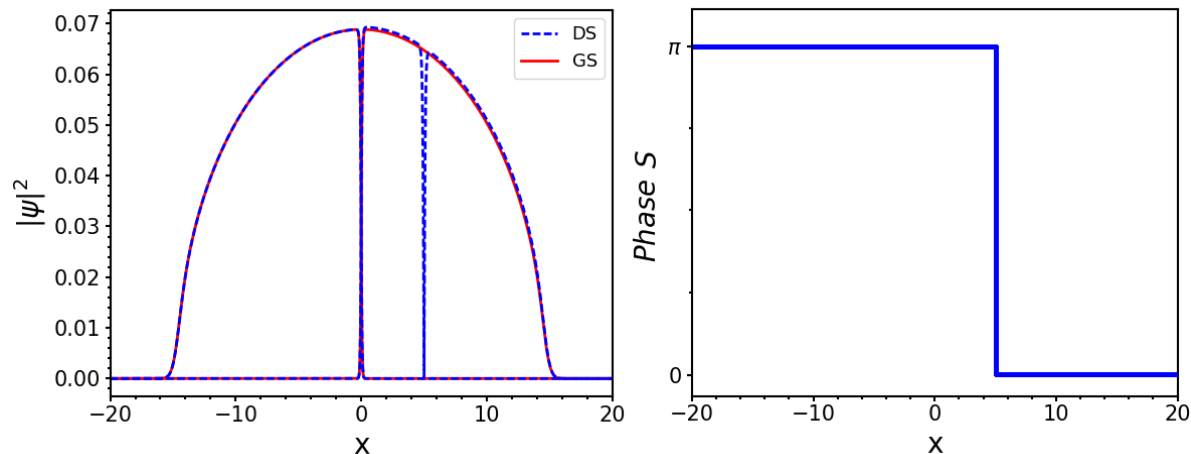

Figure 2. Left panel: density profiles of the ground state (GS) in both components (solid line) and of a dark soliton imprinted in the right component (DS) at $x = 5$ whereas the other component is in the ground state (dashed line), in a harmonic trap with $g_{11} = g_{22} = 1000$ and $g_{12} = 5000$. Right panel: phase profile of the dark soliton. All the quantities are expressed in the characteristic units of the harmonic oscillator.

Figure 2 shows the density profiles (left panel) of a dark soliton in the right component imprinted at $x = 5$ (dashed line) and the ground state (solid line) for $g_{12} = 5000$ and $g_{11} = 1000$ (all the quantities in this work are expressed in the characteristic units of the harmonic oscillator), and the phase (right panel) for the dark soliton. The phase jump ΔS of the dark soliton is π, whereas the ground state presents a constant phase (not shown) all along the condensate. One can see that confinement

plays an important role in the density profile; the trap enforces the density to go to zero at the boundary of the condensate. However, in the trapped system there exists a solitonic state even in the coupled immiscible mixture.

We can observe as well the immiscibility between the species with a small density overlap. The interphase between both components will act as a potential barrier for a particle-like object like a soliton that tries to pass through it. From the previous consideration, we expect that the soliton will achieve lower transmission coefficients in the high immiscibility regime where $g_{12}/g_{11} >> 1$.

Reflection and transmission coefficient

With the aim of studying the dynamics of a grey soliton in the interphase between both species, we have evaluated the reflection (R) and transmission (T) coefficients. We have computed the energy of each component (E_1 and E_2) and the energy of the soliton ε_s. Initially, before creating the dark soliton, the system has a total energy equal to $E^{initial} = E_1^{initial} + E_2^{initial}$. Assuming that the soliton starts moving in the first component (right component), we can define the coefficients as:

$$R = \frac{E_1^{final} - E_1^{initial}}{\varepsilon_S} \; ,$$

$$T = \frac{E_2^{final} - E_2^{initial}}{\varepsilon_S} \; , \tag{8}$$

where the *final* state corresponds to the state of the system after the first collision between the grey soliton and the interphase. It is easy to check that these definitions fulfill:

$$R + T = \frac{(E_1^{final} + E_2^{final}) - (E_1^{initial} + E_2^{initial})}{\varepsilon_S} =$$

$$= \frac{E^{final} - E^{initial}}{\varepsilon_S} = \frac{\varepsilon_S}{\varepsilon_S} = 1 \; . \tag{9}$$

We have imprinted a dark soliton in the right component at $x = 2.5$ and we have solved the two coupled GP equations (6) in real time dynamics for different immiscibility regimes. In Figure 3 we show the numerical results for the transmission coefficient of a grey soliton in a harmonic trap initially at $x = 2.5$ as a function of the ratio between the interspecies and intraspecies strength interactions. First of all, one can see that as the immiscibility between the species increases the transmission coefficient decreases. Theoretically, these systems will exhibit immiscibility behaviour when $g_{12}/g_{11} > 1$. Nonetheless, we have investigated systems deep in the immiscibility regime, so we have started with $g_{12}/g_{11} = 2$ (region II in the Figure 3), where the transmission coefficient is nearly 0.9. As we increase the strength interaction ratio, the transmission coefficient decreases exponentially until we reach an inflection point, where the value remains almost constant at 0.5. Once we pass this inflection point, the transmission coefficient
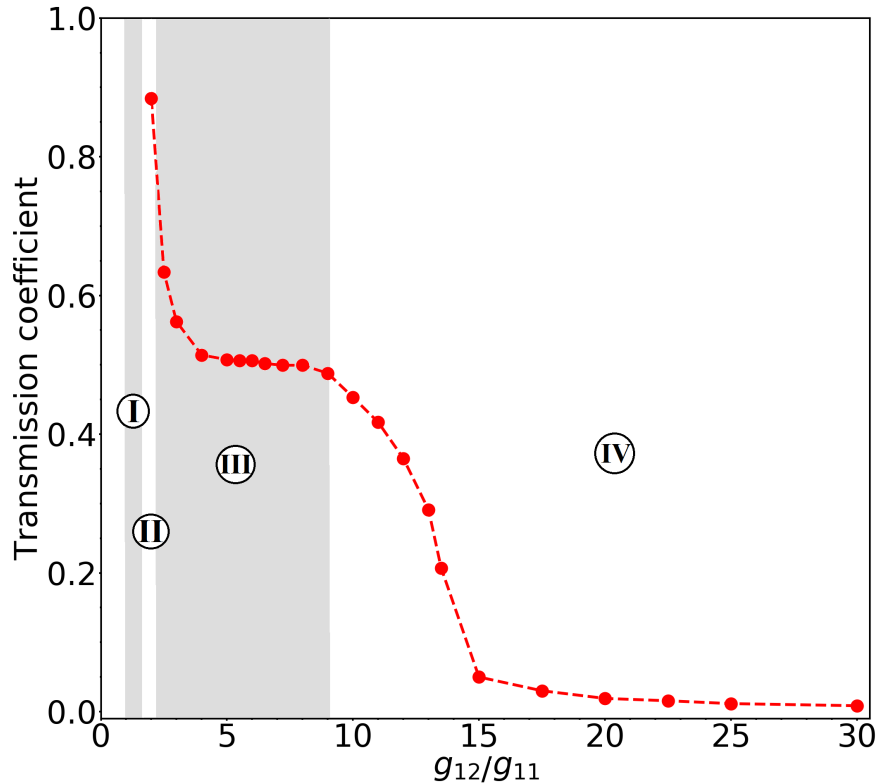
Figure 3. Transmission coefficient of the grey soliton imprinted at $x = 2.5$ in the right component as a function of the ratio between the interspecies and intraspecies strength interactions. Dashed line is a guide for the eye. We also noticed different dynamics of the soliton in the four regions plotted (I, II, III and IV).

decreases again exponentially until we reach the high immiscibility regime, where the value of the coefficient is close to 0.

We have also computed the transmission coefficients as a function of the ratio between the interspecies and intraspecies strength interactions for grey solitons with different energies, imprinting initially the soliton at different positions (the closer to the interphase the higher the energy). We have obtained similiar results as Figure 3.

In Figure 4 we show snapshots of the density profiles of both components after the dark soliton imprinted in the right component has collided with the interphase. Each panel corresponds to a different regime I, II, III and IV labelled in Figure 3. Essentially, we can distinguish four different behaviours. The first one, in the low immiscibility regime I, where the grey soliton passes through the interphase almost clean and it is transmitted to the left component without perturbations (this corresponds to a large transmission coefficient close to 1). The next regime, corresponding to II, the grey soliton also passes through the interphase, it is transmitted but one can observe the formation of a bright soliton in the right component in the density gap corresponding to the dark soliton. This gap in one component (which constitutes the component supporting the dark soliton) is filled by a bright soliton in the other component. This configuration corresponds to a dark-in-bright soliton, that were predicted theoretically
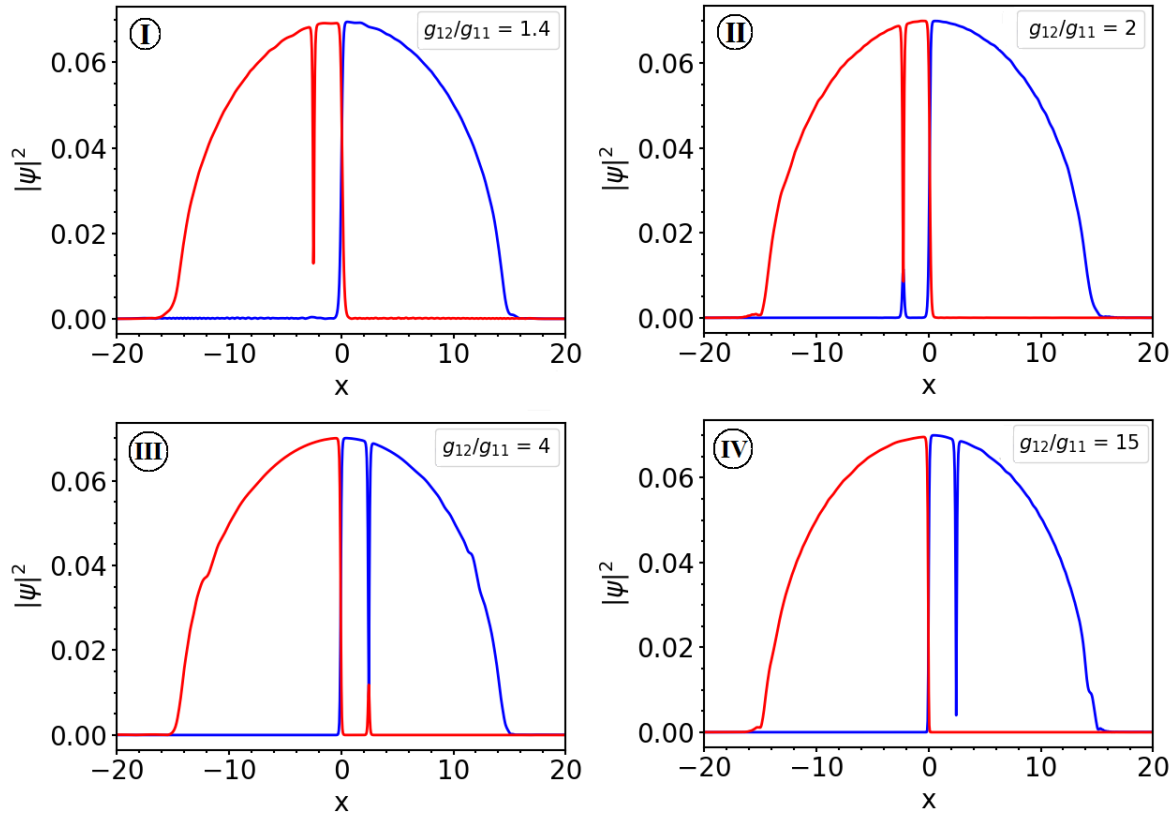
Figure 4. Snapshots of the density profiles of moving grey solitons after their first contact with the interphase between the two species. Each panel corresponds to a different regime as labelled in Figure 3.

and have been observed also experimentally two- and multiple-dark-in-bright solitons [15]. The third regime, corresponding to III, the grey soliton gets reflected once it reaches the interphase, but it creates at the same time a dark-in-bright soliton. And finally, the high immiscibility regime IV, where the dark soliton is reflected almost completely without creating a dark-in-bright soliton and the other component remains almost unaltered (the transmission coefficient tends to zero).

In order to study the stability of these solitons, we have computed a large real time evolution corresponding to ten times the period of the oscillations in the region II. It is important to stress that the solitons we have obtained are stable. Once created, the dark and bright combination does not disappear, even after each collision against the interphase, where the dark-in-bright soliton changes from one component to another.

4. Conclusions

We have analyzed the dynamical properties of a dark soliton imprinted in one component of an immiscible one dimensional mixture. Our numerical results, obtained by solving the 1D coupled Gross-Pitaeskii equations, show that as the immiscibility between the species increases the transmission coefficient decreases. Furthermore, we can

distinguish four different behaviours of the matter wave depending on the ratio between the interspecies and intraspecies strength interactions in which the soliton can be transmitted or reflected, and in between more complex dark-in-bright solitonic states can be formed. In addition, we have demonstrated that dark and dark-in-bright solitons in one dimensional harmonic trap under oscillatory motion are dynamically stable states against decay to the ground state of the system.

Acknowledgments

References

[1] A. Griffin, D. W. Snoke, and S. Stringari, *Bose-Einstein condensation*, Cambridge University Press (1995).

[2] M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman, and E. A. Cornell, *Observation of Bose-Einstein condensation in a dilute atomic vapour*, Science **269**, 198 (1995).

[3] K. B. Davies et al., *Bose-Einstein condensation in a gas of sodium atoms*, Phys. Rev. Lett. **75**, 3969 (1995).

[4] F. Dalfovo, S. Giorgini, L. P. Pitaevskii, and S. Stringari, *Theory of Bose-Einstein condensation in trapped gases*, Rev. Mod. Phys. **71**, 463 (1999).

[5] C. J. Pethick and H. Smith, *Bose-Einstein condensation in dilute gases*, Cambridge University Press (2002).

[6] C.J. Myatt, E.A. Burt, R.W. Ghrist, E.A. Cornell, and C.E. Wieman, Phys. Rev. Lett. **78**, 586 (1997).

[7] P. G. Drazin and R. S. Johnson, *Solitons: an introduction*, Cambridge University Press (1989).

[8] L. Khaykovich et al., *Formation of a matter-wave bright soliton*, Science **296**, 1290 (2002).

[9] T. Tsuzuki, J. Low Temp. Phys. **4**, 441 (1971).

[10] N. D. Mermin, *The topological theory of defects in ordered media*, Rev. Mod. Phys. **51**, 591 (1979).

[11] R. G. Scott, F. Dalfovo, L. P. Pitaevskii, and S. Stringari, Phys. Rev. Lett. **106**, 185301 (2011).

[12] S. Burger et al., *Dark solitons in Bose-Einstein condensates*, Phys. Rev. Lett. **83**, 5198 (1999).

[13] S. B. Papp, J. M. Pino, and C. E. Wieman, *Tunable miscibility in a dual-species Bose-Einstein condensate*, Phys. Rev. Lett. **101**, 040402 (2008).

[14] P. Wittek and L. Calderaro, *Massively Parallel Trotter-Suzuki Solver*, last retrieved August 2017 from `https://github.com/trotter-suzuki-mpi/trotter-suzuki-mpi`

[15] D. Yan et al., *Multiple dark-bright solitons in atomic Bose-Einstein condensates*, Phys. Rev. A **84**, 053630 (2011).