Domain Wall Solitons in Binary Mixtures of Bose-Einstein Condensates

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The structure and dynamics of the domain walls separating segregated condensates in trapped mixtures of repulsive Bose-Einstein condensates are studied. Our work reveals that, under fairly general conditions, these domain walls behave as independent dynamical entities, which allows us to identify them as constituting a novel class of multicomponent solitons in Bose-Einstein condensates.

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The recent experimental realization by Myatt *et al.* [1] of the simultaneous trapping of two distinguishable Bose-Einstein condensed gases (BECs) has paved the way in the past few years to the investigation of a new realm, namely, the physics of interacting quantum fluids. A unique feature of multispecies BECs is the presence of interspecies interactions and the resulting coupling of the different condensates. This coupling has been shown to give rise to a plethora of novel features which do not exist for pure BECs, such as complex phase diagrams [2–5], metastable states [6], vortex transfer dynamics [7,8], and symmetry breaking instabilities [4,9]. The richer dynamics occur when the coupling coefficient between two components, namely, the interspecies scattering length, is positive and large enough for these components to repel each other so as to form separate domains. In this regime, a mixture of BECs therefore exhibits a complex spatial structure, and at the heart of this organization the properties of the domain walls through which the segregated condensates interact play a dominant role [5]. The energy contribution of these domain walls is, for example, intimately related to the conditions for the occurrence of symmetry breaking [9], and the domain walls' robustness is what makes possible the existence of metastable states [6]. However, despite their importance, little attention has been paid up to now to the intimate structure of these domain walls and to their dynamical behavior. This is due to the intrinsic difficulties of describing correctly the delicate balance between particle interactions and kinetic energy that is at play at these interfaces. The aim of this Letter is to fill in this gap. In particular, our study reveals that domain walls in BECs consist of multicomponent solitons. Note that we use here the term "soliton" according to the definition of Ref. [10]. This definition states that a soliton is a stable and steady self-sustained localized structure that behaves as an independent dynamical entity in complex surroundings.

For the sake of simplicity, we will perform our analysis in the zero-temperature mean-field approximation [11]. In the two-species case, this leads to two coupled Gross-Pitaevskii (GP) equations for the macroscopic wave functions ψ_1 and ψ_2 of the condensates [2],

$$i\,\frac{\partial \psi_k}{\partial t} = \left(-\frac{m_1}{m_k}\nabla^2 + V_k(\mathbf{r}) + \sum_{l=1}^{2}\gamma_{kl}|\psi_l|^2\right)\psi_k \qquad k = 1,2\,. \tag{1}$$

These equations have been normalized by setting $\hbar = 1$ and by using $\hbar\omega_1/2$ as the energy unit and $\xi = \sqrt{\hbar/(m_1\omega_1)}$ as the length unit, where m_k and ω_k denote, respectively, the mass and trapping frequencies of each species. Also we assume that the wave functions are normalized such that $\int|\psi_k|^2\,d\mathbf{r} = N_k$, where N_k is the number of particles of species k. The coupling constants γ_{kl} are related to the three scattering lengths a_{kl} ($a_{12} = a_{21}$) representing the interactions between like and unlike particles, $\gamma_{kl} = 4\pi(a_{kl}/\xi)(m_1/\mu_{kl})$, where $\mu_{kl} = m_k m_l/(m_k + m_l)$. For brevity we shall write, in the following, a_k and γ_k, respectively, for a_{kk} and γ_{kk}. Finally, $V_k(\mathbf{r})$ are the trapping potentials in which the BECs are formed.

Since we are interested in domain walls, we consider in the following two BECs that, taken in isolation, form stable homogeneous density distributions in the absence of confining potential, $V_1 = V_2 = 0$. In other words, we consider only positive values of the scattering lengths, $\gamma_1, \gamma_2 > 0$. When two such BECs are mixed, homogeneous density distributions become unstable through symmetry breaking [4,9] and domain walls are naturally formed [5] provided that the immiscibility condition is verified. In the Thomas-Fermi approximation relevant to the present context, this condition is $\gamma_{12} > \sqrt{\gamma_1\gamma_2}$ [3,9], which simply tells us that repulsion between unlike atoms is stronger than between identical ones.

In order to show that domain walls consist of peculiar soliton solutions of the coupled GP equations (1), we first consider the one-dimensional geometry (i.e., $\partial_x = \partial_y = 0$) in the absence of confining potential ($V_1 = V_2 = 0$) and look for stationary solutions of the form $\psi_k(\mathbf{r},t) = \psi_k(z,t) = u_k(z)\exp(-i\beta_k t)$, where $u_k(z)$ and β_k are both real. Introducing these expressions into Eqs. (1) yields two ordinary differential equations which read

$$\ddot{p} = -p + p^3 + \kappa p q^2, \tag{2}$$

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$$\ddot{q} = -\beta q + \kappa^2 \gamma q^3 + \kappa p^2 q \,. \qquad (3)$$

Here $p = u_1\sqrt{\gamma_1/\beta_1}$, $q = u_2\sqrt{\gamma_1 m_1/(\beta_1 m_2)}$, and the overdots denote derivatives with respect to $z' = z\sqrt{\beta_1}$. This scaling reduces the number of parameters to two, $\kappa = (m_2\gamma_{12})/(m_1\gamma_1)$ and $\gamma = (\gamma_1\gamma_2)/\gamma_{12}^2$. $\beta = (m_2\beta_2)/(m_1\beta_1)$ is a free parameter that depends on the unknown chemical potentials β_1, β_2 of both components of the mixture. It is convenient to interpret the above equations as being the equations of motion of a unit mass in the two-dimensional potential $V(p,q) = [2(p^2 + \beta q^2 - \kappa p^2 q^2) - p^4 - \kappa^2\gamma q^4]/4$. When the two components of the mixture are immiscible (i.e., $\gamma < 1$), this potential possesses a minimum at the origin and four maxima on the p and q axes located in $p = \pm 1$, $q = 0$ and in $p = 0$, $q = \pm\sqrt{\beta/(\kappa^2\gamma)}$. These maxima correspond to uniform (i.e., z-independent) stationary single-component solutions of the GP equations (1) with $V_1 = V_2 = 0$. In the mechanical analog picture, the unit mass can leave such a maximum to go down the potential, cross the minimum at the origin, and reach the opposite maximum [cf. the separatrix trajectory shown as a dotted line in Fig. 1(a)]. Since the motion to leave the maximum (as well as to reach the opposite one) takes an infinite "time" z, the corresponding inhomogeneous solution $[p(z), q = 0]$ or $[p = 0, q(z)]$ represents a localized structure of the atomic density. It is easy to verify from Eqs. (2) and (3) that this localized structure is nothing but the well-known tanh-shaped dark soliton of single-component BECs that was recently observed experimentally [12]. If the free parameter satisfies $\beta = \sqrt{\kappa^2\gamma}$, the potential takes the same value for adjacent maxima, namely, $V = 1/4$. In this case, adjacent maxima are separated by a saddle point where $V < 1/4$. As a consequence, separatrix trajectories exist that connect pairs of adjacent maxima. Since they link homogeneous stationary single-component solutions of the two species, such separatrices correspond to new multicomponent BEC solitons. These solitons consist of stationary localized structures separating two homogeneous BECs of different immiscible species. The coupled GP equations being in general nonintegrable, we have calculated their soliton solutions numerically. The separatrix of the first quadrant is shown in Fig. 1(a) together with the contour lines of the potential V in the case $\gamma = 0.4$ and $\kappa = 1.83$. The corresponding soliton $p(z')$, $q(z')$ is shown in Fig. 1(b).

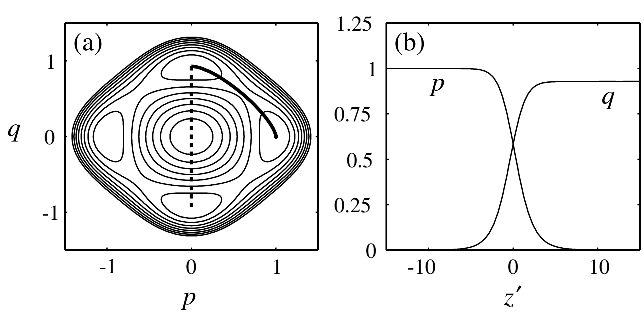

FIG. 1. (a) Contour lines of the potential $V(p,q)$ and the separatrix trajectories between two opposite (dotted line) and adjacent (solid line) maxima for $\gamma = 0.4$ and $\kappa = 1.83$. (b) The domain wall soliton corresponding to the trajectory between adjacent maxima.

Such domain wall solitons (DWS) were already identified in the context of nonlinear optics [13,14]. In particular, DWS were shown to exist in association with optical vortices [14], exhibiting behaviors similar to what has been observed in BECs [7,8]. A connection between DWS and modulational instability [13] was also revealed that can be associated with the instabilities existing in the low energy excitation spectra of multispecies BECs [6]. To address fully the soliton nature of the domain walls in BEC mixtures, however, we must investigate how the trapping potentials affect their structure and behavior. Moreover, DWS have so far been described only in one- and two-dimensional geometries [13,14]. It is therefore important to study their existence in the three-dimensional case that is relevant to BECs.

Before going further, we must point out that, in order for the DWS to be observable in practice, the BEC confinement must be such that the width of the domain wall is smaller than the spatial extension of the BEC. This condition is not trivial and it is therefore important to evaluate the width of DWS for practical experimental parameters. To perform a realistic evaluation, suitable pairs of atomic states must first be selected. For DWS to exist, we require that the three scattering lengths characterizing the mixture be positive and that the interspecies interaction be sufficiently repulsive to have $\gamma < 1$. Moreover, the inelastic collision rate between the two species must be sufficiently small for the condensates to live long enough to be created and probed. A very interesting candidate is a mixture of $^{87}\mathrm{Rb}|1,-1\rangle$ and $^{85}\mathrm{Rb}|2,2\rangle$. The inelastic cross section is very small and both the interspecies scattering length and the scattering length of $^{85}\mathrm{Rb}|2,2\rangle$ can be controlled by applying a bias magnetic field, taking advantage of Feshbach resonances [15,16]. This mixture can actually sustain DWS with values of γ that can be tuned between 0 and 1. Given these properties, we will further investigate this mixture in the following, referring to it as mixture A; species 1 and 2 are $^{87}\mathrm{Rb}|1,-1\rangle$ and $^{85}\mathrm{Rb}|2,2\rangle$, respectively ($a_1 = 5.66$ nm, $a_2 = 0\ldots20$ nm, $a_{12} \simeq 10.5$ nm, $\kappa = 1.83$). Among mixtures made of different hyperfine states of the same isotope, the only candidate is a mixture of the states $|1,-1\rangle$ and $|2,1\rangle$ (or $|2,2\rangle$) of ^{87}Rb because other isotopes suffer large spin-exchange collision losses [17]. This mixture exhibits, however, a value of $\gamma \simeq 0.999$, very close to the critical value of 1 [18] and it is actually not clear whether or not $\gamma < 1$. Nevertheless, we include a discussion of this case in our Letter because it will yield some insights into the role of the confining potential and because this mixture is the only one that has been realized experimentally up to now [1,18]. We will refer to it as mixture B, the states $|1,-1\rangle$ and $|2,1\rangle$ being, respectively, species 1 and 2 ($a_1 = 5.66$ nm, $a_2 = 5.33$ nm, $a_{12} = 5.495$ nm, $\kappa = 0.97$).

Let us now evaluate the widths w of DWS and check that the solitons can be hosted in a realistic trapped BEC. w is conveniently expressed as a function of the particle density, $w \sim \Delta z' (8\pi a_1 |\psi|^2)^{-1/2}$, where $\Delta z'$ is the dimensionless width of the DWS calculated from Eqs. (2) and (3). $|\psi|^2$ is the average particle density of the condensates that can be easily calculated for practical experimental parameters using the Thomas-Fermi approximation [11]. Considering the BEC made up of 5×10^5 atoms of ^{87}Rb described in Ref. [19], we find a trapped cloud diameter $d \sim 30 \mu$m and a particle density $|\psi|^2 \sim 5 \times 10^{19}/\mathrm{m}^3$. This yields the condition $\Delta z' \ll 80$ for the DWS to be comfortably hosted in the BEC. Our calculations reveal that this condition is satisfied for the mixture A provided that $\gamma < 0.95$ ($\Delta z' < 20$) but not for the mixture B, for which we have $\Delta z' \simeq 140$. In this latter case, the repulsion between the two species is very weak (i.e., γ is very close to 1) so that the two components of the mixture overlap over a large region and the corresponding DWS are very broad. We therefore anticipate that DWS are unlikely to be observed in this mixture unless there is an increase in the effective interactions between the two components by trapping a very large number of atoms or by using a strongly anisotropic trap. This result also reveals that the current generation of experiments dealing with multispecies BECs [1,18,19] cannot provide any clues as to the existence of DWS in binary BECs as they were all performed with mixture B in near-isotropic trapping conditions.

To gain further insights into the behavior of the domain walls in trapped BECs, the GP equations (1) with harmonic trapping potentials have been solved numerically. We first considered a one-dimensional model because it makes possible a simple and direct comparison with the exact DWS solution (i.e., the DWS associated with domains of infinite extent) of Eqs. (2) and (3). Of course, with this 1D model the number of particles N_k are defined somewhat arbitrarily. In practice, we used the same number of particles $N_1 = N_2 = 8000$ for both mixtures A and B so as to highlight the differences between them. The results are presented in Figs. 2 and 3. Figure 2(a) shows the particle distribution for a trapped mixture A with $\gamma = 0.2$. We can observe a close agreement between the profile of the domain walls that separate the two trapped BECs and the exact DWS solution (dotted lines). This agreement could be expected because here the width of the domain walls is much smaller than the overall size of the condensate. The solitonic nature of the domain walls that separate the two components of the mixture can be further revealed through the analysis of their dynamics. In the context of optics, DWS were shown to be extremely robust and to behave as independent dynamical entities [13]. This solitonic nature can be remarkably well illustrated in the present context by applying a strong perturbation to the particle distribution of the trapped mixture of Fig. 2(a). We perturb the system by removing the right-hand sidelobe of species 1. The subsequent evolution is shown in Fig. 2(b). As can be seen, the domain wall is perfectly preserved while both particle distributions undergo strong oscillations. Numerous other numerical simulations with time-dependent potential parameters have shown the same independence of the domain walls width with respect to the BEC's overall dynamics. The situation is quite different with mixture B for which the exact DWS are much larger than the trapped BEC [Fig. 3(a)]. Here, the particle distribution cannot be related to DWS. In particular, we have verified that the shape of the condensates does not change when increasing γ up to 1.001, for which DWS do not exist. The existence of a dip in the distribution of species 1 as observed in Fig. 3(a) as well as in experiments [18] appears, however, quite counterintuitive. Indeed, the size of the exact DWS (shown by the dotted lines in Fig. 3) that gives the spatial scale at which the atomic species repulse each other is clearly larger than the BEC width itself. We would therefore anticipate the formation of a homogeneous mix of the two species instead of two seemingly repulsing BECs, as shown in Fig. 3(a). This feature can be explained by considering that the atom distribution is here mainly determined by the trapping potentials. By strongly confining one species in the center of the trap, the trap is able to effectively enhance the interspecies interaction so as to force the other species to distribute itself on an outer shell. This predominant role of the trapping potentials is confirmed by Fig. 3(b) which shows the dramatic redistribution of the atoms when the trap centers seen by the two species

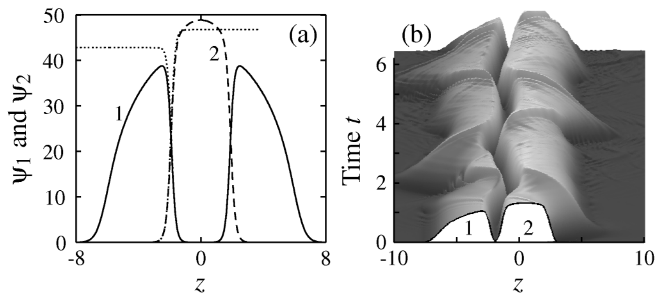

FIG. 2. (a) Mixture A in a one-dimensional trapping potential ($N_1 = N_2 = 8000$, $\gamma = 0.2$). The dotted lines show the exact DWS. (b) Three-dimensional plot showing the evolution of the mixture after removing the right-hand sidelobe of species 1. Both distributions have been separated by opposite translations of $1/2$ in z so as to make the edges of the DWS clearly visible.

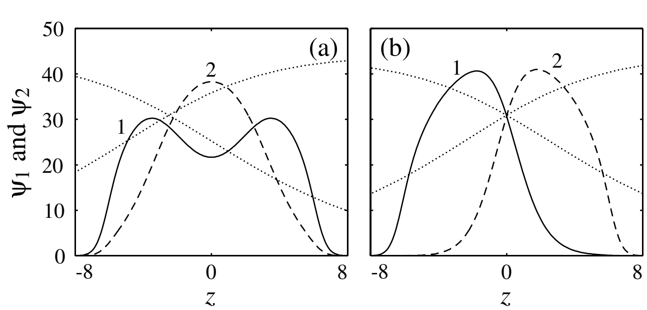

FIG. 3. Mixture B in a one-dimensional trapping potential ($N_1 = N_2 = 8000$). The dotted lines show the exact DWS. In (b) the trap centers have been shifted by $\delta z = \pm 0.1$.

are slightly shifted with respect to each other, a feature which has been observed experimentally [18]. The relative shift of the two traps $\delta z = \pm 0.1$ is here smaller than 1% of the total width of the mixture. Such a high sensitivity to the trap positions is not observed with mixture A, therefore confirming that no DWS are at play in mixture B for the number of particles considered here.

A better control of the shape and density of trapped BECs can be obtained by taking advantage of the additional degrees of freedom provided by a more realistic three-dimensional trapping geometry. DWS could in this way be observed in mixture B with a reasonable number of particles (provided that γ is indeed smaller than the critical value of 1). We anticipate that a cigar-shaped trap would be an ideal candidate for such an experiment. The tight confinement in the transverse plane increases the particle densities, therefore enhancing the interactions between the particles, while the weak confinement in the orthogonal direction leads to a long atom cloud that provides plenty of space to host DWS. To investigate this configuration, we looked numerically for the ground-state solution of the GP equations (1) for the full three-dimensional geometry with trapping potentials of the form $V_k = m_k \omega_k^2 [x^2 + \lambda(y^2 + z^2)]/2$. The results of such a calculation with a mesh of $60 \times 60 \times 60$ points are shown in Fig. 4 in the case of mixture B with $\gamma = 0.999$, $N_1 = N_2 = 10^7$, and a trap anisotropy parameter $\lambda = 316$. Figure 4(a) provides a three-dimensional representation of the isosurfaces of the two components of the mixture while 4(b) shows the atomic population densities along the line $y = z = 0$, i.e., along the weakly confined direction. We observe a symmetric distribution of the atoms with two clear-cut domain walls separating the two species. Since the cigar-shaped trap geometry is in essence quasi-one-dimensional, this solution can still be compared with the exact DWS solution [dotted lines in 4(b)] of Eqs. (2) and (3). The close agreement observed suggests that the atom distribution along the x axis is now essentially governed by DWS and no longer by the trapping potentials.

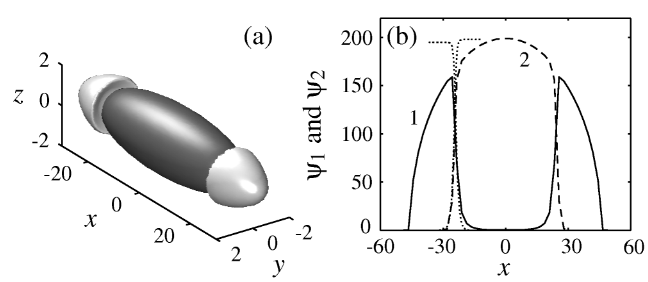

FIG. 4. Mixture B in a three-dimensional cigar-shaped trap. The isosurfaces of the wave functions at level 130 are plotted in (a) (light and dark gray correspond, respectively, to species 1 and 2) while (b) represents the atomic densities of both species along the line $y = z = 0$. The dotted lines show the exact one-dimensional DWS.

Further three-dimensional calculations with various mixtures, number of particles, and different values of the critical coefficient γ revealed that domain wall solutions are not peculiar to the two mixtures exemplified in this Letter. Provided that γ is not too close to the critical value of 1 (say, $\gamma < 0.95$), the soliton nature of the domain walls in trapped BEC mixtures already reveals itself with 10^5 atoms of each species. This leads us to conclude that the recognition of the domain walls in BEC mixtures as truly independent dynamical entities could become important for the interpretation of the next generation experiments on two-component dilute BECs. Moreover, we anticipate that DWS may also play an important role in the dynamics of more complicated BEC mixtures such as optically trapped spinor condensates [3]. Finally, from a more fundamental point of view, our work also constitutes the first study of the existence and stability of three-dimensional domain wall solitons.

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[1] C. J. Myatt *et al.,* Phys. Rev. Lett. **78**, 586 (1997).
[2] T.-L. Ho and V. B. Shenoy, Phys. Rev. Lett. **77**, 3276 (1996).
[3] J. Stenger *et al.,* Nature (London) **396**, 345 (1998).
[4] P. Öhberg and S. Stenholm, Phys. Rev. A **57**, 1272 (1998).
[5] E. Timmermans, Phys. Rev. Lett. **81**, 5718 (1998).
[6] H. Pu and N. P. Bigelow, Phys. Rev. Lett. **80**, 1134 (1998).
[7] M. R. Matthews *et al.,* Phys. Rev. Lett. **83**, 2498 (1999).
[8] J. J. García-Ripoll and V. M. Pérez-García, Phys. Rev. Lett. **84**, 4264 (2000).
[9] B. D. Esry and C. H. Greene, Phys. Rev. A **59**, 1457 (1999).
[10] V. E. Zakharov, *Physical Encyclopedia,* edited by A. M. Prokhorov (Great Russian Encyclopedia, Moscow, 1994); V. G. Makhankov, Phys. Rep. **35**, 1 (1978).
[11] F. Dalfovo, S. Giorgini, L. P. Pitaevskii, and S. Stringari, Rev. Mod. Phys. **71**, 463 (1999).
[12] S. Burger *et al.,* Phys. Rev. Lett. **83**, 5198 (1999).
[13] M. Haelterman and A. P. Sheppard, Phys. Rev. E **49**, 3389 (1994); M. Haelterman, Electron. Lett. **31**, 741 (1995).
[14] A. P. Sheppard and M. Haelterman, Opt. Lett. **19**, 859 (1994).
[15] J. P. Burke, Jr., J. L. Bohn, B. D. Esry, and C. H. Greene, Phys. Rev. Lett. **80**, 2097 (1998).
[16] S. L. Cornish *et al.,* Phys. Rev. Lett. **85**, 1795 (2000).
[17] P. S. Julienne, F. H. Mies, E. Tiesinga, and C. J. Williams, Phys. Rev. Lett. **78**, 1880 (1997).
[18] D. S. Hall *et al.,* Phys. Rev. Lett. **81**, 1539 (1998).
[19] M. R. Matthews *et al.,* Phys. Rev. Lett. **81**, 243 (1998).