

# Binary mixtures of condensates in generic confining potentials

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## Abstract

We study a binary mixture of Bose–Einstein condensates, confined in a generic potential, in the Thomas–Fermi approximation. We search for the zero-temperature ground state of the system, both in the case of fixed numbers of particles and fixed chemical potentials. For generic potentials, we analyze the transition from mixed to separated ground-state configurations as the inter-species interaction increases. We derive a simple formula that enables one to determine the location of the domain walls. Finally, we find criteria for the energetic stability of separated configurations, depending on the number and the position of the domain walls separating the two species.

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(Some figures may appear in colour only in the online journal)

## 1. Introduction

Binary mixtures of Bose–Einstein condensates are of great interest due to their complex dynamical features and their role in the emergence of macroscopic quantum phenomena. Mixtures are usually made up of two species that can also be hyperfine states of the same alkali atom [1]. They generally display repulsive self-interaction and are confined by different potentials. Depending on the inter-species interaction, two classes of stable configurations are possible: mixed and separated. The latter are more interesting, since they allow the observation of phenomena such as symmetry breaking, e.g., in harmonic potentials and macroscopic quantum tunneling [2, 3]. Binary mixtures in harmonic traps have been investigated in a number of interesting experiments [4–6].

Different approaches are possible in order to study the ground state of these systems. The binary mixture of two species of bosons can be rigorously described in a second-quantization formalism [7]. However, if the number of particles in the condensate is very large compared to the number of particles in the excited states, the fields associated with the two species can be treated as classical wavefunctions. This approach leads to the Gross–Pitaevskij (GP) equations

[8] that are obtained by minimizing the zero-temperature grand-canonical energy of the system. The ground state of the system can be thus determined by solving the GP equation [9–12], or equivalently by analytically or numerically minimizing the grand-canonical energy functional [2, 3, 13]. Analytical results are obtained only in particular cases, such as confinement by a hard wall trap [14], harmonic or lattice potentials [15] and axisymmetric traps [16], also in the presence of the gravitational force [17]. A simplified approach is often used, based on the Thomas–Fermi (TF) approximation, that consists in neglecting the kinetic energy with respect to the self- and inter-species interaction energies [8]. This reduces the problem of finding the ground state of the binary mixture of condensates to a classical problem, related to the stability of a system of two interacting fluids.

In this paper, we shall investigate this problem by adopting the following approach: given a system of two interacting condensates, confined in a generic external potential (that can be different for the two species), we will find *general* tools to determine the ground state of such a system in the TF approximation. The paper has the following structure. In section 2, we set up the problem and introduce notation. In section 3, we find a threshold value of the inter-species interaction parameter, above which mixed configurations cannot be the ground state of the system. In section 4, we establish those conditions that determine which one of the possible separated configurations is the ground state. We conclude with an outlook in section 5. Throughout this paper, both cases of (i) fixed numbers of particles and (ii) fixed chemical potentials will be considered.

## 2. Gross–Pitaevskij equations and Thomas–Fermi solutions

We consider a system made up of two species of indistinguishable particles, labeled 1 and 2, confined by generally different external potentials  $V_1(x)$  and  $V_2(x)$ . Self-interaction and inter-species interaction are assumed to be repulsive. An example of such a system is a mixture of alkali atoms in two different hyperfine states [4, 5]. The two subsystems are described in a quantum field theoretical framework, by associating with each species the field operators  $\hat{\psi}_1(x)$  and  $\hat{\psi}_2(x)$ . However, since we are searching for the zero-temperature ground state, we assume that all particles condense in the same wavefunction, and thus apply a Bogoliubov shift [18] and treat  $\psi_1(x)$  and  $\psi_2(x)$  as classical fields, normalized to the average numbers of particles  $N_1$  and  $N_2$ . The grand-canonical energy functional is

$$\mathcal{E} = \mathcal{T} + \mathcal{U} - \mu_1(\mathcal{N}_1 - N_1) - \mu_2(\mathcal{N}_2 - N_2), \quad (1)$$

where

$$\begin{aligned} \mathcal{T} &= \int \left( \frac{\hbar^2}{2m_1} |\nabla \psi_1|^2 + \frac{\hbar^2}{2m_2} |\nabla \psi_2|^2 \right) d^m x, \\ \mathcal{U} &= \int \left( V_1 |\psi_1|^2 + V_2 |\psi_2|^2 + \frac{U_{11}}{2} |\psi_1|^4 + \frac{U_{22}}{2} |\psi_2|^4 + U_{12} |\psi_1|^2 |\psi_2|^2 \right) d^m x, \end{aligned} \quad (2)$$

$$\mathcal{N}_k = \mathcal{N}(|\psi_k|^2) = \int |\psi_k(x)|^2 d^m x, \quad k = 1, 2$$

and  $m$  is the dimension of the system. By requiring that the energy is stationary, one obtains the coupled GP equations

$$\left( -\frac{\hbar^2}{2m_1} \Delta + V_1(x) + U_{11} |\psi_1(x)|^2 + U_{12} |\psi_2(x)|^2 \right) \psi_1(x) = \mu_1 \psi_1(x), \quad (3)$$

$$\left( -\frac{\hbar^2}{2m_2} \Delta + V_2(x) + U_{22} |\psi_2(x)|^2 + U_{12} |\psi_1(x)|^2 \right) \psi_2(x) = \mu_2 \psi_2(x). \quad (4)$$

In the above equations  $U_{11}$  and  $U_{22}$  are the self-interaction parameters between atoms of the same species, while  $U_{12}$  is associated with inter-species interaction. Each of these parameters is assumed to be positive, since we are considering repulsive interactions. The solutions of (3) and (4) depend on the value of the chemical potentials  $\mu_1$  and  $\mu_2$ , which are Lagrange multipliers. If  $\mu_1$  and  $\mu_2$  are fixed, the average particle numbers are free to vary. If, on the other hand, the particle numbers  $N_1$  and  $N_2$  are fixed, the chemical potentials are chosen in such a way that the wavefunctions satisfy the normalization constraints  $\mathcal{N}_k = N_k$ , for  $k = 1, 2$ .

For the sake of simplicity, our analysis will be focused on one-dimensional systems, with the main results generalizable to higher dimensions. Moreover, it will be assumed that the potentials be continuously differentiable,  $V_k \in C^1(\mathbb{R})$ . This class of potentials schematizes very well those used in trapping cold atoms.

The TF approximation, which will be applied in the following, consists in neglecting the kinetic energy contribution  $\mathcal{T}$  to the energy functional (1). This approximation is justified if the numbers of particles in the system are sufficiently large. More precisely, in three-dimensional traps the TF approximation is applicable if the parameter  $N_k a_k$ , where  $a_k$  is the s-wave scattering length of species  $k$ , is very large compared with the typical trapping length  $a_T (= \sqrt{\hbar/m\omega_{\text{ho}}})$  for a harmonic trap of frequency  $\omega_{\text{ho}}$ . In standard experimental configurations,  $a_k/a_T$  is typically of order  $10^{-3}$  [8], and thus  $N_k$  is of order  $10^{4-6}$  (see [19] for a single condensate and [4–6] for a mixture), ensuring that the parameter  $N_k a_k/a_T$  is indeed large, and thus the TF approximation is valid. In one-dimensional configurations, one should require that  $N_k a_k a_\ell/a_\perp^2 \gg 1$ , where  $a_\ell$  and  $a_\perp$  are the longitudinal and transverse trapping lengths, respectively, provided  $N_k$  and  $a_k$  are not large enough to excite the transverse degrees of freedom. A realization of a quasi-one-dimensional Bose system was achieved in [20], where a highly anisotropic harmonic potential of frequencies  $\omega_\perp = 2\pi \times 360$  Hz and  $\omega_\ell = 2\pi \times 3.5$  Hz traps sodium atoms (s-wave scattering length  $a = 2.8$  nm). In this case, the one-dimensional TF applicability condition is already verified if the number of atoms is  $10^{3-4}$ .

Under these conditions, for a single condensate, as  $N_k$  increases, the kinetic energy contribution to (1) becomes vanishingly small with respect to both the potential and interaction energy  $E_{\text{TF}}$  [8]. For binary mixtures, another relevant contribution to the kinetic energy can arise if the density profiles have rapidly varying parts, corresponding to *domain walls* sharply separating the two species. This extra term is due to the exponential penetration of one species into the other one through the domain wall [21], but it results in  $O(N_k^{-1/2})$  with respect to the self-interaction energies, and can thus be neglected as a first approximation for large  $N_k$ .

The TF approximation provides a very accurate tool to determine the ground-state density profiles of single condensate and mixtures. Nonetheless, the kinetic energy plays an important role for finite  $N_k$  in the case of binary mixtures, by limiting the number of domain walls. Thus, the TF approximation is a good starting point for very large numbers of particles.

As a consequence of the TF approximation, the grand-canonical energy becomes dependent only on the densities  $\rho_1(x) = |\psi_1(x)|^2$  and  $\rho_2(x) = |\psi_2(x)|^2$ , and will be indicated in the following as  $\mathcal{E}_{\text{TF}}(\rho_1, \rho_2)$ .

Note that, without loss of generality, one can reduce the analysis to the particular case  $U_{11} = U_{22} = 1$ . Indeed, by scaling

$$\rho_k \rightarrow \rho_k/\sqrt{U_{kk}}, \quad N_k \rightarrow N_k/\sqrt{U_{kk}}, \quad V_k \rightarrow V_k\sqrt{U_{kk}}, \quad \mu_k \rightarrow \mu_k\sqrt{U_{kk}} \quad (5)$$

one obtains

$$\mathcal{E}_{\text{TF}}(\rho_1, \rho_2) = \mathcal{U}(\rho_1, \rho_2) - \mu_1(\mathcal{N}(\rho_1) - N_1) - \mu_2(\mathcal{N}(\rho_2) - N_2), \quad (6)$$

with

$$\mathcal{U}(\rho_1, \rho_2) = \frac{1}{2} \int (\rho_1^2 + \rho_2^2 + 2\alpha\rho_1\rho_2) dx + \int (V_1\rho_1 + V_2\rho_2) dx \quad (7)$$

and

$$\alpha = \frac{U_{12}}{\sqrt{U_{11}U_{22}}}. \quad (8)$$

Incidentally, note that the above reduction to a single parameter  $\alpha$  applies also to the full energy functional (1), by also scaling the masses  $m_k \rightarrow m_k/\sqrt{U_{kk}}$ .

The critical points of the TF grand-canonical energy functional are the solutions to the algebraic equations

$$\rho_1(x) + \alpha\rho_2(x) + V_1(x) = \mu_1, \quad \rho_2(x) + \alpha\rho_1(x) + V_2(x) = \mu_2 \quad (9)$$

and will be called the TF density profiles. Moreover, for fixed particle numbers  $N_k$ , they are supplemented by the normalization conditions

$$\int \rho_k dx = N_k, \quad k = 1, 2, \quad (10)$$

which fix the values of the chemical potentials  $\mu_k$ .

In the following, the supports of the TF densities  $\rho_k$  will be denoted by  $S_k$ . By assuming that  $\alpha \neq 1$ , in  $S_{12} = S_1 \cap S_2$ , where both condensates are present, the TF density profiles are

$$\rho_1(x) = \frac{\mu_1 - V_1(x) - \alpha(\mu_2 - V_2(x))}{1 - \alpha^2}, \quad \rho_2(x) = \frac{\mu_2 - V_2(x) - \alpha(\mu_1 - V_1(x))}{1 - \alpha^2}. \quad (11)$$

In the regions  $S_{11} = S_1 - S_2$  and  $S_{22} = S_2 - S_1$ , occupied by only one of the two species, the solutions are respectively

$$\rho_1(x) = \mu_1 - V_1(x), \quad \rho_2(x) \equiv 0, \quad (12)$$

and

$$\rho_2(x) = \mu_2 - V_2(x), \quad \rho_1(x) \equiv 0. \quad (13)$$

The TF density profiles (11)–(13) are defined independently of the dimensionality of the system.

Note that the TF equations (9) uniquely determine the functional dependence of the densities at a point  $x$  on the external potentials at the same point, the chemical potentials and the interaction parameters, *once* the supports  $S_1$  and  $S_2$  are given. On the other hand, large freedom is left in the choice of the supports of the density profiles, for which uniqueness fails. Thus, extremely irregular configurations can be solutions of the TF equations. Among all possible solutions, one should pick up the minimizers.

The rest of this paper will be devoted to deriving general rules for finding the minimizing configuration of the supports, in order to determine the ground state of the system, both if the numbers of particles and the chemical potentials are fixed.

### 3. Mixed versus separated configurations

The configurations of the binary mixture can be divided into two fundamental parts: separated and mixed. The TF densities are *mixed* in  $S_{12} = S_1 \cap S_2$ , where both species are present, and are *separated* in  $S_{11} \cup S_{22} = S_1 \cup S_2 - S_1 \cap S_2$ , where only one species is present at one time. A configuration is said to be separated if it does not contain mixed parts, and mixed otherwise. We proceed by treating separately the two cases (i) fixed numbers of particles and (ii) fixed chemical potentials.

### 3.1. Solutions are confined

We will first prove that under the assumption that the  $C^1$  potentials are confining, i.e.

$$V_k(x) \rightarrow +\infty, \quad \text{for } |x| \rightarrow \infty, \quad (14)$$

with  $k = 1, 2$ , all TF density profiles are compactly supported. We will see that this is a straight consequence of the positivity of the densities

$$\rho_k(x) \geq 0. \quad (15)$$

We will prove that the supports  $S_k$  are bounded, by separately considering the sets with separated phases,  $S_{11} = S_1 - S_2$  and  $S_{22} = S_2 - S_1$ , and that with mixed phases,  $S_{12} = S_1 \cap S_2$ . By requiring that the solutions (12) and (13) be non-negative we obtain

$$\begin{aligned} S_{11} &\subset \{x \in \mathbb{R} \mid V_1(x) \leq \mu_1\} = V_1^{-1}(-\infty, \mu_1], \\ S_{22} &\subset \{x \in \mathbb{R} \mid V_2(x) \leq \mu_2\} = V_2^{-1}(-\infty, \mu_2], \end{aligned} \quad (16)$$

which are bounded by hypothesis. On the other hand, from (11) we obtain that every point  $x \in S_{12}$  satisfies the conditions

$$\frac{\mu_1 - V_1(x) - \alpha(\mu_2 - V_2(x))}{1 - \alpha^2} \geq 0, \quad \frac{\mu_2 - V_2(x) - \alpha(\mu_1 - V_1(x))}{1 - \alpha^2} \geq 0. \quad (17)$$

They are easily proved to be equivalent to

$$\min\{\alpha, \alpha^{-1}\}(\mu_2 - V_2(x)) \leq (\mu_1 - V_1(x)) \leq \max\{\alpha, \alpha^{-1}\}(\mu_2 - V_2(x)), \quad (18)$$

which in turn imply that

$$S_{12} \subset V_1^{-1}(-\infty, \mu_1] \cap V_2^{-1}(-\infty, \mu_2], \quad (19)$$

so that  $S_{12}$  is compact. As a consequence,  $S_1 = S_{11} \cup S_{12}$  and  $S_2 = S_{22} \cup S_{12}$  are compact.

### 3.2. Fixed numbers of particles

If the numbers of particles  $N_1$  and  $N_2$  are kept fixed, the chemical potentials are functionally dependent on the density profiles, since they have to be tuned in order to preserve the normalization conditions (10). The search for the zero-temperature ground state of the system reduces to the minimization of the TF grand-canonical energy functional (6) that, evaluated at the TF solutions, reduces to the internal energy functional (7).

*3.2.1. Square well.* We start from the well-known case study of a binary mixture confined in a square well, corresponding to a bounded interval of the real axis  $S = [a, b]$  (with  $b > a$ ). This example will be proved useful in the following.

The internal energy of a completely mixed configuration is fixed by the TF prescription for the density profiles (with  $V_k(x) \equiv 0$ ) and the normalization conditions. On the other hand, the energy of a separated configuration with  $N_1$  particles of the first species in a subset  $S_1 \subset S$  and  $N_2$  particles of the second in  $S_2 = S - S_1$  is a function of the length  $|S_1|$ . It can be easily verified (see e.g. [8]) that the minimization of the internal energy of a separated configuration is attained for supports  $\bar{S}_1$  and  $\bar{S}_2 = S - \bar{S}_1$  (corresponding to densities  $\bar{\rho}_1$  and  $\bar{\rho}_2$ ) verifying

$$\frac{N_1}{|\bar{S}_1|} = \frac{N_2}{|\bar{S}_2|} \quad (\iff \quad \bar{\rho}_1 = \bar{\rho}_2). \quad (20)$$

Since the difference between the internal energy of the optimal separated configuration  $\mathcal{U}_s$  and the one of the mixed configuration  $\mathcal{U}_m$  reads

$$\Delta\mathcal{U} = \mathcal{U}_s - \mathcal{U}_m = \frac{N_1 N_2}{b - a} (1 - \alpha), \quad (21)$$

the minimizing separated configurations are energetically favored if  $\alpha \geq 1$ , while the mixed configurations are less energetic than all separated configurations if  $\alpha < 1$ . For a binary mixture in a square well, this proves the well-known role of

$$\alpha^{\text{th}} = 1 \quad (U_{12}^{\text{th}} = \sqrt{U_{11}U_{22}}) \quad (22)$$

as a threshold value.

*3.2.2. Selection principle and regularity of solutions.* Note that the minimizers have a very high degeneracy, since every sets  $\tilde{S}_1$  whose measures satisfy (20) correspond to possible TF configurations. Among them, despite the regularity of the potentials, there are extremely irregular configurations with highly entangled supports and infinitely many points of discontinuity (domain walls). However, such a phenomenon is a consequence of the TF approximation that, by neglecting the kinetic energy part  $\mathcal{T}$  in (1), is also deprived of its regularizing effect on the densities. The kinetic term favors smooth density profiles. Indeed, due to the presence of the kinetic energy, the grand-canonical energy functional (1) is defined on functions with square integrable (distribution) derivatives, and TF solutions are approximations thereof. In particular, in the one-dimensional situation, a domain wall is a discontinuous approximation of a (absolutely) continuous function that changes between two values in a very short transition region with a large derivative.

Thus, each domain wall of the TF solution would correspond to an additional cost, in terms of kinetic energy of the true solution, and the above-mentioned degeneracy would be lifted; among the TF degenerate minimizers,  $\mathcal{T}$  would select those one(s) with the minimum number of domain walls. In the following, we will make use of this *selection principle* and, in particular, we will only consider densities in the class of piecewise differentiable functions,  $\rho_k \in \tilde{C}^1$ . This means that there is a finite subdivision of  $S_k$  such that the restriction of  $\rho_k$  to each subinterval  $[t_j, t_{j+1}]$  is continuously differentiable. Incidentally, note that the potentials themselves can be assumed to be piecewise differentiable, without modifying our results.

Going back to the square-well case, by the selection principle, for  $\alpha \geq 1$ , we end up with only two degenerate minimizers: one with  $S_1 = [a, c]$ , where  $c = (aN_2 + bN_1)/(N_1 + N_2)$ , and the other with  $S_1 = [d, b]$ , where  $d = (aN_1 + bN_2)/(N_1 + N_2)$ . Both configurations are separated and have a single domain wall.

*3.2.3. Generic potential.* We now extend the above result to the case in which the mixture is not confined in a square well, but rather by generic continuously differentiable confining potentials  $V_k(x)$  with  $k = 1, 2$ . We will prove that, if  $\alpha \geq 1$ , the ground state of the system is a separated configuration, and thus we can restrict our attention to the separated ones.

Let the TF densities have a mixed configuration in  $S_{12} = S_1 \cap S_2$ , given by equation (11). Since the densities  $\rho_k$  are assumed to be piecewise continuously differentiable, and their supports are compact,  $S_{12}$  is the union of a finite number of compact intervals in which the  $\rho_k$  are  $C^1$ . Choose a segment  $\omega = [x_0, x_1]$  of length  $|\omega| = \varepsilon > 0$  included in some of those intervals. The interval  $\omega$  contains

$$n_j = \int_{\omega} \rho_k(x) dx = \varepsilon \langle \rho_k \rangle \quad (k = 1, 2) \quad (23)$$

particles, where  $\langle \cdot \rangle$  denotes the average on  $\omega$ . Since the potentials are  $C^1$ , we can express them in  $\omega$  as

$$V_k(x) = V_k(x_0) + V'_k(\xi_k(x))(x - x_0), \quad k = 1, 2, \quad (24)$$

for some  $\xi_k(x) \in \omega$ .

Since the  $\rho_k$  are continuous in  $\omega$ , two points  $\bar{x}_k$  exist in this segment, in which the functions equal their averages:

$$\rho_k(\bar{x}_k) = \langle \rho_k \rangle. \quad (25)$$

Moreover, since the density functions are continuously differentiable in  $[x_0, x_1]$ , taking into account (25) we can express them in each point of the segment as

$$\rho_k(x) = \langle \rho_k \rangle + \rho'_k(\eta_k(x))(x - \bar{x}_k), \quad (26)$$

for some  $\eta_k(x) \in \omega$ . The first derivatives appearing in (24)–(26) are all bounded in  $\omega$ . Thus, the internal energy of particles in the set  $\omega$  reads

$$u_m = \varepsilon \left[ \frac{1}{2} \langle \rho_1 \rangle^2 + \frac{1}{2} \langle \rho_2 \rangle^2 + \alpha \langle \rho_1 \rangle \langle \rho_2 \rangle + V_1(x_0) \langle \rho_1 \rangle + V_2(x_0) \langle \rho_2 \rangle \right] + \mathcal{O}(\varepsilon^2). \quad (27)$$

We now divide  $\omega$  into two subintervals  $\omega_1 = [x_0, y]$  and  $\omega_2 = [y, x_1]$ :

$$\omega = \omega_1 \cup \omega_2, \quad (28)$$

and replace the TF mixed densities in  $\omega$  with flat and separated density profiles, preserving the particle numbers

$$\bar{\rho}_1 = \frac{n_1}{|\omega_1|} \quad \text{for } x \in \omega_1, \quad (29)$$

$$\bar{\rho}_2 = \frac{n_2}{|\omega_2|} \quad \text{for } x \in \omega_2. \quad (30)$$

As a rule in choosing the bipartition of  $\omega$ , we assume that the stationarity condition (20) for the internal energy in an infinite potential well is satisfied

$$\frac{|\omega_2|}{|\omega_1|} = \frac{n_2}{n_1}. \quad (31)$$

Taking into account the result (21), concerning the self-interaction and inter-species interaction parts, the potential energy of the set  $\omega$  with separated densities (29)–(30) can be expressed, after a straightforward manipulation, as

$$u_s = \varepsilon \left[ \frac{1}{2} \langle \rho_1 \rangle^2 + \frac{1}{2} \langle \rho_2 \rangle^2 + \langle \rho_1 \rangle \langle \rho_2 \rangle + V_1(x_0) \langle \rho_1 \rangle + V_2(x_0) \langle \rho_2 \rangle \right] + \mathcal{O}(\varepsilon^2). \quad (32)$$

The net change in the total potential energy, due to the replacement of the mixed densities in  $[x_0, x_1]$  with the separated ones, is

$$\delta\mathcal{U} = u_s - u_m = \varepsilon (1 - \alpha) \langle \rho_1 \rangle \langle \rho_2 \rangle + \mathcal{O}(\varepsilon^2). \quad (33)$$

For sufficiently small  $\varepsilon$ , the sign of  $\delta\mathcal{U}$  is determined by the first term in (33), unless  $\alpha = 1$ .

If  $\alpha > 1$ , the result  $\delta\mathcal{U} < 0$  implies that, given a point of a mixed configuration, there always exists a neighborhood in which one can construct a separated configuration with lower energy. Since  $S_{12}$  is compact, we can find a finite subdivision  $S_{12} = [x_0, x_1] \cup \dots \cup [x_{n-1}, x_n]$ , such that the above construction can be performed in each segment  $[x_{j-1}, x_j]$ . Thus, the minimizers are separated configurations, if the particle numbers are fixed. Analogously, one can show that if  $\alpha < 1$  the internal energy of a separated configuration is always larger than the energy of a mixed configuration with the same particle numbers. Thus, even in the case of varying external potentials, the value (22) acts as a threshold between mixed and separated ground states.

### 3.3. Fixed chemical potentials

If the chemical potentials  $\mu_1$  and  $\mu_2$  are fixed, the average particle numbers are free to vary. In order to find the ground state of the system, one has to find the minimizers of the grand-canonical energy  $\mathcal{E}_{\text{TF}}(\rho_1, \rho_2)$ . As in the case of fixed particle numbers, the elementary case of a binary mixture in an infinite square well will be analyzed first. Then, we will try and find general results in the case of different piecewise continuously differentiable confining potentials.

*3.3.1. Square well.* It is clear from (11)–(13) that fixing the chemical potentials corresponds to fixing the density functions, with the choice of the supports leading to different numbers of particles. We will neglect a nonessential annoying constant in (6) by setting  $N_1 = N_2 = 0$ .

In the simple case of an infinite square well  $S$  with  $V_1 = V_2 = 0$  inside the well, the only values of the chemical potentials that have physical meaning are the positive ones, as it emerges from (16) and (19). In the following, we shall set  $\mu_2 \leq \mu_1$  without loss of generality. Let us first consider a completely mixed configuration in the well with density profiles

$$\rho_1^m = \frac{\mu_1 - \alpha\mu_2}{1 - \alpha^2}, \quad \rho_2^m = \frac{\mu_2 - \alpha\mu_1}{1 - \alpha^2}. \quad (34)$$

Such a configuration has a physical meaning if both densities are non-negative. Thus, if  $\alpha < 1$  the numerators in (34) must be non-negative, while if  $\alpha > 1$  the numerators must be non-positive. Conditions on the positivity of the densities set a bound on the values of  $\alpha$  which are compatible with the chosen chemical potentials:

$$\alpha \notin \left( \frac{\mu_2}{\mu_1}, \frac{\mu_1}{\mu_2} \right). \quad (35)$$

The problem of non-physical values of  $\alpha$  does not arise in the case

$$\mu_2 = \mu_1, \quad (36)$$

which will prove to be a very relevant physical situation. If (36) holds, the boundaries (35) coincide, and the densities are well defined for all  $\alpha$ . Note that condition (36) exactly corresponds to the minimum condition of the internal energy in the separated phase, since, by taking into account (12)–(13), it implies  $\rho_1^s = \rho_2^s$ .

If the solutions (34) are plugged in the definition of the grand-canonical energy, it is possible to express it in terms of interaction parameters and chemical potentials:

$$\mathcal{E}_m = |S| \left[ \frac{\mu_1^2 + \mu_2^2 - 2\mu_1\mu_2\alpha}{2(\alpha^2 - 1)} \right]. \quad (37)$$

If instead separated solutions are considered, with the first condensate confined in a region  $S_1$  and the second in  $S_2 = S - S_1$ , the grand-canonical energy is a function of the length  $|S_1|$  and reads

$$\mathcal{E}_s(|S_1|) = -|S_1| \frac{\mu_1^2}{2} - |S - S_1| \frac{\mu_2^2}{2}. \quad (38)$$

Since (38) is linear in the length  $|S_1|$ , it is clear that its minimum value is

$$\bar{\mathcal{E}}_s = -|S| \frac{\mu_1^2}{2}. \quad (39)$$

Hence, if  $\mu_2 < \mu_1$  the minimum of the grand-canonical energy for separated configurations corresponds to  $S_1 = S$ . (In the same way, if  $\mu_2 > \mu_1$ , it corresponds to  $S_2 = S$ .) In this case, the minimizer is in fact a *single condensate* configuration. Only if (36) holds, separated configurations are allowed. Moreover, their energy is stationary with respect to changes in the partition of  $S$ .

The energy in the mixed configuration and that in the minimizing separated configuration will now be compared in detail. In the case  $\mu_2 < \mu_1$ , for  $0 \leq \alpha < \mu_2/\mu_1$  energy  $\mathcal{E}_m$  (37) increases, but it is always lower than  $\bar{\mathcal{E}}_s$ , and thus the TF ground state corresponds to the mixed configuration. For  $\mu_2/\mu_1 \leq \alpha \leq \mu_1/\mu_2$ , separated configurations (not only the minimizing one) are the only ones that have a physical meaning. In the range  $\alpha > \mu_1/\mu_2$ , the mixed configurations become physical again, but their energy that vanishes like  $\alpha^{-1}$  for  $\alpha \rightarrow \infty$  is always greater than  $\bar{\mathcal{E}}_s$ ; thus, the TF ground state is the configuration with a single condensate (of species one).

We now consider the case  $\mu_2 = \mu_1$ . It was observed that this is the only case in which real separated states minimize the grand-canonical energy  $\mathcal{E}_s$ , and thus it is possible for such configurations to be the ground state of the system. By plugging condition (36) into equation (37), we find that the grand-canonical energy of the mixed configuration reads

$$\mathcal{E}_m = -|S| \frac{\mu_1^2}{1 + \alpha}. \quad (40)$$

If (40) is compared with  $\bar{\mathcal{E}}_s$  in equation (38), mixed configurations are found to be favored if  $\alpha < 1$ , while separated configurations have smaller energy if  $\alpha > 1$ . Thus, even in the case of fixed chemical potentials, with  $\mu_1 = \mu_2$ , and infinite square-well external potential, the value (22) proves to be the discriminant value between mixed and separated ground states.

**3.3.2. Generic potential.** Consider TF density profiles  $\rho_k(x)$ . In  $S_{11} = S_1 - S_2$ , we obtain (with the convention  $N_1 = N_2 = 0$ )

$$\mathcal{E}_s^{(1)} = \frac{1}{2} \int_{S_{11}} (\mu_1 - V_1)^2 dx - \int_{S_{11}} (\mu_1 - V_1)^2 dx = -\frac{1}{2} \int_{S_{11}} (\mu_1 - V_1)^2 dx \quad (41)$$

and in  $S_{22} = S_2 - S_1$

$$\mathcal{E}_s^{(2)} = -\frac{1}{2} \int_{S_{22}} (\mu_2 - V_2)^2 dx. \quad (42)$$

Therefore,

$$\mathcal{E}_s = -\frac{1}{2} \int_{S_{11}} \tilde{V}_1(x)^2 dx - \frac{1}{2} \int_{S_{22}} \tilde{V}_2(x)^2 dx, \quad (43)$$

with

$$\tilde{V}_k(x) = \mu_k - V_k(x) \quad (k = 1, 2). \quad (44)$$

In  $S_{12} = S_1 \cap S_2$ , we obtain

$$\mathcal{E}_m = -\frac{1}{2(1 - \alpha^2)} \int_{S_{12}} (\tilde{V}_1(x)^2 + \tilde{V}_2(x)^2 - 2\alpha \tilde{V}_1(x)\tilde{V}_2(x)) dx. \quad (45)$$

Compare a mixed TF configuration in a set  $S$  with a configuration with only one species, say  $\rho_1$ ,

$$\begin{aligned} \delta\mathcal{E} &= \mathcal{E}_s^{(1)} - \mathcal{E}_m = \frac{1}{2} \int_S \tilde{V}_1^2 dx + \frac{1}{2(1 - \alpha^2)} \int_S (\tilde{V}_1^2 + \tilde{V}_2^2 - 2\alpha \tilde{V}_1 \tilde{V}_2) dx \\ &= -\frac{1}{2(1 - \alpha^2)} \int_S (\tilde{V}_2 - \alpha \tilde{V}_1)^2 dx. \end{aligned} \quad (46)$$

Thus, when  $\alpha > 1$  one obtains  $\delta\mathcal{E} \leq 0$  and separated configurations are energetically favored. Therefore, in this condition, we have to search for the ground state among the separated configurations, which is the aim of the following section.

### 3.4. Remarks

From the results obtained in this section, it clearly emerges that, if  $\alpha \geq 1$ , that is,  $U_{12} \geq U_{12}^{\text{th}}$ , the ground state is in a separated configuration. Moreover, according to the selection principle introduced in section 3.2.2, the following analysis will be restricted to piecewise continuously differentiable solutions of the TF equations,  $\rho_k \in \tilde{C}^1$ , whose discontinuities can be due to the presence of a finite number of interfaces.

#### 4. Minimizing separated configurations

In section 3, it was shown that separated configurations are energetically favored if

$$\alpha > 1, \tag{47}$$

for generic continuously differentiable confining potentials. We will now find a way to determine which of these configurations is the ground state of the system, and which can be regarded to be locally stable or unstable. We shall again discuss separately the cases of fixed numbers of particles and fixed chemical potentials, underlining analogies and differences between them.

When only piecewise continuously differentiable density profiles are considered, a separated configuration can be characterized by the property that the supports  $S_1$  and  $S_2$  do not intersect, except at a finite set of points. The intersection points correspond to a set of domain walls separating the first and the second species.  $S_1$  and  $S_2$ , being compact, are thus unions of intervals, which can be bounded by (i) two domain walls, (ii) a domain wall and a zero of the TF density profile, or (iii) two zeros. From (12) and (13), the possible zeros  $\xi_j^{(k)}$ , with  $j = 1, \dots, m$  and  $k = 1, 2$ , of the densities  $\rho_k$  are subject to the condition

$$\mu_k = V_k(\xi_j^{(k)}). \tag{48}$$

In general, if we search the ground state among the separated configurations, we have to deal with the minimization of the sum of two decoupled functionals of the kind

$$\mathcal{U}(\rho_1, \rho_2) = \mathcal{V}(\rho_1) + \mathcal{V}(\rho_2). \tag{49}$$

We remark that, except for condition (47) that enables one to establish that the ground state is a separated configuration, the parameter  $\alpha$  plays no role in the search for minimal separated configurations.

We will proceed by fixing the number  $n$  of domain walls and determine the set of positions  $\vec{R} = (R_1, \dots, R_n)$  for which the considered functional, internal or grand-canonical energy, is, at least locally, minimized. We will then compare the minima corresponding to different numbers of walls.

##### 4.1. Fixed numbers of particles

In this case, our aim is to find the stationary configurations of the internal energy

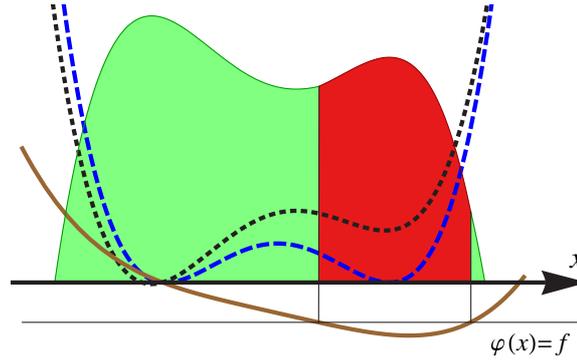
$$\mathcal{U}(\rho_1, \rho_2) = \frac{1}{2} \int_{S_1} (\rho_1(x)^2 + 2V_1(x)\rho_1(x)) dx + \frac{1}{2} \int_{S_2} (\rho_2(x)^2 + 2V_2(x)\rho_2(x)) dx \tag{50}$$

with respect to small variations of  $\vec{R}$ , under the condition that the numbers of particles  $N_k$  remain fixed,  $\int_{S_k} \rho_k dx = N_k$ . Then, conditions will be set for these stationary configurations to be local minima. It can easily be inferred that the chemical potentials in (12) and (13), which are used as Lagrange multipliers to normalize the density profiles and thus depend on the supports  $S_1$  and  $S_2$ , are the functions of the domain wall positions  $\vec{R}$ . We re-express the separated TF density profiles, explicitly showing this additional dependence:

$$\rho_k(x; \vec{R}) = \mu_k(\vec{R}) - V_k(x) \quad (k = 1, 2). \tag{51}$$

The zeros  $\xi_j^{(k)}$ , subject to condition (48), are also functions of  $\vec{R}$ . Since the choice of the position of the domain walls completely defines the density profiles and their supports, the internal energy (50), evaluated at stationary TF densities, can be viewed as a function of  $\vec{R}$ :

$$\mathcal{U}(\rho_1(\cdot; \vec{R}), \rho_2(\cdot; \vec{R})) := U(\vec{R}). \tag{52}$$



**Figure 1.** Stationary configuration for a binary mixture of two species confined in different external potentials. The (blue) dashed line represents the external potential  $V_1(x)$  and the (black) dotted line potential  $V_2(x)$  in arbitrary units. The (brown) solid line is the difference  $\varphi(x) = V_1(x) - V_2(x)$  that appears in equation (55). The density profile of the first species is in dark gray (red in the online version), while the density profile of the second one is in light gray (green in the online version). All the plotted quantities are rescaled according to equation (5). As prescribed by the condition (54), the densities  $\rho_1$  and  $\rho_2$  at the edges of domain walls are equal. The domain walls are placed at those points where the function  $\varphi(x)$  has the same value.

We now assign to each domain wall a dichotomic variable  $s_j$ :  $s_j = +1$  if it is the upper border of an interval containing the first species (and thus the lower border of an interval containing the second one) and  $-1$  in the complementary case.

By taking the first derivative of (52) with respect to a generic  $R_j$  and using normalization conditions, one obtains

$$\frac{\partial U(\vec{R})}{\partial R_j} = \frac{s_j}{2} (\rho_2(R_j; \vec{R})^2 - \rho_1(R_j; \vec{R})^2). \tag{53}$$

The stationarity condition is obtained by setting to zero the derivatives (53) with respect to all the positions of the  $n$  domain walls, yielding

$$\rho_1(R_j; \vec{R}) = \rho_2(R_j; \vec{R}) \quad \forall j = 1, \dots, n. \tag{54}$$

These are clearly analogous to the minimum conditions (20) in the case of an infinite potential well. If the densities in (54) are expressed as functions of the external potentials and the chemical potentials, it becomes clear that the position of the domain walls in a stationary configuration is characterized by the fact that the potential

$$\varphi(x) := V_1(x) - V_2(x) \tag{55}$$

is equal for all  $R_j$ :

$$\varphi(R_j) = \mu_1(\vec{R}) - \mu_2(\vec{R}). \tag{56}$$

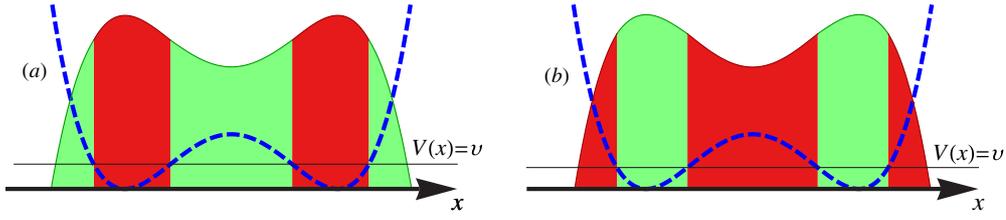
Let us consider the equation

$$\varphi(x) = f, \tag{57}$$

with  $f$  a constant. The number of its solutions fixes the maximal number of walls in a stationary configuration. An example of stationary configuration for different confining potentials is reported in figure 1.

The case in which the external potentials for the two species are proportional is particularly interesting:

$$V_2(x) = \beta V_1(x) =: \beta V(x), \tag{58}$$



**Figure 2.** Examples of maximal stationary configurations in a symmetric double-well potential. The (blue) dashed line represents the external potential  $V_1(x) \equiv V(x)$ , confining particles of first species, in arbitrary units. Particles of the second species are subjected to the potential  $V_2(x) = \sqrt{U_{11}/U_{22}} V(x)$ , with  $U_{11} < U_{22}$ . This situation corresponds to equal physical (not scaled) trapping potentials. The density profile of the first species is in dark gray (red in the online version), while the density profile of the second one is in light gray (green in the online version). The scaled densities at the edges of a domain wall satisfy condition (54). In (a), the minima of the potential are occupied by the first species, which is the less self-interacting one. In (b), the minima are occupied by the second species. It is evident that the domain walls in both stationary configurations (a) and (b) are placed at points with the same value of the potential  $V(x)$  (see equation (60)). Computation of the second derivatives shows that, since  $U_{11} < U_{22}$ , only configuration (a) is (at least locally) stable.

with  $\beta > 0$ . This occurs, e.g., when the two condensates feel the same potential before the scaling (5), and in such a situation

$$\beta = \sqrt{\frac{U_{11}}{U_{22}}}. \quad (59)$$

In the case of proportional potentials (58), equation (57) specializes to

$$V(x) = v, \quad (60)$$

with  $v$  being a constant. If (60) has at most  $n$  solutions, there cannot exist stationary configurations with more than  $n$  domain walls. In this case, the domain walls are placed at positions characterized by the same potential, which must be equal to

$$V(R_j) = \frac{\mu_1(\vec{R}) - \mu_2(\vec{R})}{1 - \beta}, \quad \forall j = 1, \dots, n. \quad (61)$$

As a consequence, the densities of the same species must be equal at the edge of each domain wall. The values of the densities at the edge of all domain walls in the case of proportional potentials will be indicated as  $\tilde{\rho} = \rho_1(R_j) = \rho_2(R_j)$ .

Henceforth, we shall call *maximal stationary configurations* those ones in which a domain wall is placed in each of the real solutions of (61), except for the case in which one of the solutions is a stationary point for  $V(x)$ . Two different examples of such configurations are shown in figure 2. In the following, it will be shown that for  $\beta \approx 1$  the ground state of the system is usually in a maximal configuration.

In order to determine if the stationary configurations are in fact minima of (52), the Hessian matrix  $H$  at the stationary solution has to be computed. By deriving (53) once more with respect to  $R_j$ , we find that  $\partial^2 U / \partial R_j^2$  has two contributions: the first one is related to the dependence of the external potentials on the point  $R_j$  and the second one to the dependence of the chemical potentials on the position of the domain walls  $\vec{R}$ . On the other hand, if (53) is derived with respect to  $R_k$  with  $j \neq k$ , only the second one of the above-mentioned contributions survives. By taking into account conditions (54), the diagonal elements of the Hessian matrix in the

stationary configurations read

$$H_{jj} = s_j \rho_1(R_j; \vec{R}) \varphi'(R_j) + \left( \frac{1}{|S_1|} + \frac{1}{|S_2|} \right) \rho_1(R_j; \vec{R})^2, \quad (62)$$

while the non-diagonal elements are

$$H_{jk} = s_j s_k \left( \frac{1}{|S_1|} + \frac{1}{|S_2|} \right) \rho_1(R_j; \vec{R}) \rho_1(R_k; \vec{R}). \quad (63)$$

For a large number of particles, so that  $|S_k|$  are sufficiently large, all terms depending on the inverse length can be neglected, and conditions for the Hessian matrix are positive definite, and hence for the corresponding stationary configuration to be a local minimum, are easy to find

$$\begin{aligned} \varphi'(R_j) > 0 &\Leftrightarrow V'_1(R_j) > V'_2(R_j) && \text{if } s_j = +1, \\ \varphi'(R_j) < 0 &\Leftrightarrow V'_1(R_j) < V'_2(R_j) && \text{if } s_j = -1. \end{aligned} \quad (64)$$

For smaller numbers of particles, the complete Hessian matrix has to be diagonalized (e.g. in a numerical way). A simpler and relevant case is that of equal external potentials, in which we have already remarked that in a stationary configuration the values of the densities of each species must be equal at all the domain walls. We obtain

$$H_{jk}^{\text{pp}} = \delta_{jk} a_j + (-1)^{j+k} C, \quad (65)$$

where we have taken into account that  $s_j s_k = (-1)^{j+k}$  and defined

$$a_j = s_j \tilde{\rho} (1 - \beta) V'(R_j) \quad (66)$$

as the intensive and purely diagonal part, and

$$C = \left( \frac{1}{|S_1|} + \frac{1}{|S_2|} \right) \tilde{\rho}^2 \quad (67)$$

as the length-dependent term, which vanishes for large numbers of particles. In this limit, when  $\beta < 1$  the condition for a stationary configuration to be locally stable is that the potential  $V(x)$  be increasing at *all* the  $R_j$  that are the upper (right) border of an interval containing particles of the first species ( $s_j = +1$ ), and decreasing at *all* the  $R_j$  that are the lower (left) border of an interval of the same kind ( $s_j = -1$ ). Intuitively, the less self-interacting condensate (since we supposed that  $\beta < 1$  in equation (59)) tends to occupy regions of the real axis in which the potential is lower, while the most self-interacting one is pushed into regions where the external potential is higher. For small numbers of particles, such configurations continue to be minima for (52), since if the potential is increasing when  $s_j = +1$  and decreasing when  $s_j = -1$ ,  $H_{jk}^{\text{pp}}$  in equation (65) is the sum of two positive definite matrices, and hence it is positive definite. Moreover, it is possible that even a configuration in which

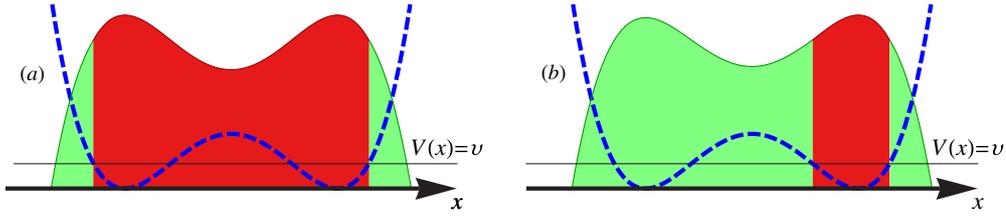
$$a_j \leq 0 \quad \text{for some } j \in \{1, \dots, n\} \quad (68)$$

becomes stable, which is impossible in the thermodynamic limit. However, bounds on the stability of such configurations can be found if some necessary conditions for (65) to be positive definite are tested. First, since  $|H_{ij}^{\text{pp}}| \leq (H_{ii}^{\text{pp}} + H_{jj}^{\text{pp}})/2$  for all pairs of indices, then

$$a_i + a_j \geq 0, \quad \forall i, j = 1, \dots, n, \quad (69)$$

which implies that only one of the  $\{a_j\}$ , say  $a_{\bar{j}}$ , can be non-positive for a stable configuration, and moreover

$$|a_{\bar{j}}| \leq \min_{j \neq \bar{j}} a_j. \quad (70)$$



**Figure 3.** Non-maximal configurations in a double-well potential. Lines and shades have the same meaning as in figure 2. Both configurations refer to the case  $U_{11} < U_{22}$ . In (a), the first species occupies a region around the potential barrier, where the potential is higher than its value in the domain walls. In (b), the second species occupies the region around one of the minima of the external potential, where it is lower than its value in correspondence of the domain walls. Although locally stable, density profiles (a) and (b) are *not* ground states.

On the other hand, by applying the necessary condition  $\det H > 0$ , another constraint can be established,

$$|a_{\bar{j}}| < \frac{C}{1 + C \sum_{j \neq \bar{j}} a_j^{-1}}, \quad (71)$$

with the upper bound vanishing in the thermodynamic limit.

There are two kinds of maximal stationary configurations: the first one is characterized by the fact that the external potential at each point of  $S_1$  is smaller than the potential at each point of  $S_2$ , while the second one is characterized by the opposite situation. The latter, however, is not stable, since the diagonal part of its Hessian matrix contains  $a_i < 0$  for all  $i = 1, \dots, n$ . We can thus limit our attention to the first kind of profiles, which we call the *maximal stable configurations* (see figure 2). We will now prove that if a locally stable configuration is not maximal, there are conditions ensuring that it cannot be the ground state of the system. The proof is based on the fact that in a non-maximal and locally stable configuration one of the following situations emerges: either the potential at a point of  $S_1$  is greater than the potential at the domain walls or the potential at a point of  $S_2$  is smaller than its value at the domain walls. Examples of non-maximal configurations are represented in figure 3. We remark that both these situations can be present in the same configuration. We start by considering the first one. Let

$$v = V(R_j) \quad (72)$$

be the potential at the domain walls. Assume that the potential at a point  $x_0 \in S_1$  be such that

$$V(x_0) =: \bar{V}_1 > v. \quad (73)$$

We exclude the case  $\bar{V}_1 = \mu_1$ , implying a vanishing density at  $x_0$ . (This case will be eventually considered as a limit.) We now consider a subinterval  $\omega_\epsilon$  of  $S_2$  of length  $\epsilon > 0$ , with a domain wall as one of its edges, and an interval  $\omega_\eta$  of length  $\eta > 0$ , which is a neighborhood of  $x_0$ , and impose that the number of first-species particles in  $\omega_\eta$  be equal to  $n_0$  and that of second-species particles in  $\omega_\epsilon$  be  $n_0/\beta$ . Since the potential is regular and the densities are supposed to be regular between each pair of domain walls, one obtains

$$n_0 = \eta \rho_1(x_0) + O(\eta^2) = \epsilon \beta \rho_2(R_j) + O(\epsilon^2). \quad (74)$$

This equality implies a relation between the length of the considered intervals, depending on the ratio of the densities, which can be expressed in terms of the potentials by using condition (54):

$$\eta(\epsilon) = \epsilon \beta \frac{\rho_2(R_j)}{\rho_1(x_0)} + O(\epsilon^2) = \epsilon \beta \frac{\mu_1 - v}{\mu_1 - \bar{V}_1} + O(\epsilon^2). \quad (75)$$

The potential energy of the two selected intervals is given by the sum of the contributions

$$u_\epsilon^{(2)} = vn_0 + \frac{1}{2} \frac{n_0^2}{\epsilon\beta^2} + O(\epsilon^2), \quad (76)$$

$$u_\eta^{(1)} = \bar{V}_1 n_0 + \frac{1}{2} \frac{n_0^2}{\eta(\epsilon)} + O(\epsilon^2). \quad (77)$$

We now replace the original density profiles with flat density profiles which preserve the numbers of particles. In particular, we fill  $\omega_\epsilon$ , which initially belonged to  $S_2$ , with the first-species condensate with a density

$$\bar{\rho}_1 = \frac{n_0}{\epsilon}, \quad (78)$$

and  $\omega_\eta$  with the second-species particles with a density

$$\bar{\rho}_2 = \frac{n_0}{\eta(\epsilon)\beta}. \quad (79)$$

With these new density profiles, the internal energy of the intervals becomes the sum of the terms

$$u_\epsilon^{(1)} = vn_0 + \frac{1}{2} \frac{n_0^2}{\epsilon} + O(\epsilon^2), \quad (80)$$

$$u_\eta^{(2)} = \bar{V}_1 n_0 + \frac{1}{2} \frac{n_0^2}{\eta(\epsilon)\beta^2} + O(\epsilon^2). \quad (81)$$

The total variation of the internal energy induced by this change is

$$\delta\mathcal{U} = u_\epsilon^{(1)} + u_\eta^{(2)} - u_\epsilon^{(2)} - u_\eta^{(1)} = \frac{n_0^2}{2} \left( \frac{1}{\beta^2} - 1 \right) \left( \frac{1}{\eta(\epsilon)} - \frac{1}{\epsilon} \right) + O(\epsilon^2). \quad (82)$$

Since  $\beta < 1$ , we find that if  $\eta(\epsilon) > \epsilon$ , i.e. up to first order in  $\epsilon$ ,

$$\frac{\mu_1 - v}{\mu_1 - \bar{V}_1} > \frac{1}{\beta}, \quad (83)$$

and it is always possible, for sufficiently small  $\epsilon$ , to find a density profile that preserves the numbers of particles, whose energy is smaller than the energy of a non-maximal stable configuration. It can be observed that if the limit  $\bar{V}_1 \rightarrow \mu_1$  is taken, condition (83) is certainly satisfied. This means that in the ground-state configuration the intervals of the support  $S_1$  of the less self-interacting species cannot be bordered by a zero.

If the case in which there exists a point in  $x_0 \in S_2$ , where the external potential is lower than its value in the domain walls,

$$V(x_0) =: \bar{V}_2 < v, \quad (84)$$

we find, with the same procedure as in the previous case, that if the following inequality is satisfied:

$$\frac{\mu_2 - v}{\mu_2 - \bar{V}_2} < \beta, \quad (85)$$

then the considered non-maximal configuration can never be the ground state of the system. Since usually  $\beta^2 = U_{11}/U_{22} \simeq 1$  (see, e.g., the hyperfine states of  $^{87}\text{Rb}$ , [2]), conditions (83)–(85) set a very stringent limitation on the possibility that a non-maximal stable configuration can be the ground state of the binary mixture.

#### 4.2. Fixed chemical potentials

The results in the case of fixed chemical potentials are very similar to that of fixed numbers of particles in the thermodynamical limit. The functional to be minimized by the separated configuration is (we set  $N_1 = N_2 = 0$ )

$$\mathcal{E}(\rho_1, \rho_2) = \int_{S_1} \left( \frac{1}{2} \rho_1^2 + V_1 \rho_1 - \mu_1 \rho_1 \right) dx + \int_{S_2} \left( \frac{1}{2} \rho_2^2 + V_2 \rho_2 - \mu_2 \rho_2 \right) dx. \quad (86)$$

An important difference with respect to the previous case is that, since the chemical potentials are fixed and not subject to normalization conditions, the TF density functions are completely independent of the positions of the domain walls. Thus, the functional (86) depends on  $\vec{R}$  only through the domains of integrations, which are determined by the supports of the density profiles, and it can be seen again as a function of the domain wall positions:

$$\mathcal{E}(\rho_1(\cdot; \vec{R}), \rho_2(\cdot; \vec{R})) := E(\vec{R}). \quad (87)$$

The stationarity conditions are exactly the same as in the case of fixed numbers of particles, since the first derivative with respect to a generic  $R_j$  reads

$$\frac{\partial E(\vec{R})}{\partial R_j} = \frac{s_j}{2} (\rho_2(R_j; \vec{R})^2 - \rho_1(R_j; \vec{R})^2). \quad (88)$$

However, the Hessian matrix in the stationary configurations is diagonal, as in (62). The absence of the non-diagonal part lies in the fact that the first derivative (88) depends on the position of the domain walls only through the external potentials. The stability criteria for a stationary density profile are the same as in the case of fixed numbers of particle, if the thermodynamical limit is considered: a configuration is stable if and only if conditions (64) are satisfied for all  $j$ . If the two species lie in the same external potential, these conditions reduce to  $s_j V'(R_j) > 0$ .

Even in the case of fixed chemical potentials, it is possible to show that if the potentials are proportional (58), there are limitations on the possibility that a non-maximal stable configuration can be the ground state. Indeed, if at the domain walls we have  $V(R_j) = v$ , it can be shown that if there exists a point in  $S_1$ , where the potential is  $\bar{V}_1 > v$  and satisfies

$$\frac{\mu_2 - \bar{V}_1}{\mu_1 - \bar{V}_1} > \frac{1}{\beta}, \quad (89)$$

then the grand-canonical energy of the configuration is higher than the energy of another configuration corresponding to the same chemical potentials. We observe that the stationarity condition (54) (with the chemical potentials *independent* of  $\vec{R}$ ) implies that the chemical potential  $\mu_2$  is greater than  $\mu_1$ . Thus, the left-hand side of (89) is an increasing function of  $\bar{V}_1$ . Moreover, the equality is saturated for  $\bar{V}_1 = v$ . We remark that if the limit  $\bar{V}_1 \rightarrow \mu_1$  is considered, that is if the density profile of the first-species condensate has a zero, condition (89) is certainly verified, and then such a configuration cannot be the ground state of the system. On the other hand, if there exists a point in  $S_2$  where the potential is  $\bar{V}_2 < v$ , satisfying

$$\frac{\mu_1 - \bar{V}_2}{\mu_2 - \bar{V}_2} > \beta, \quad (90)$$

then there exists another configuration corresponding to the same chemical potentials, which has a lower grand-canonical energy. In this second case, the left-hand side of (90) is a decreasing function of  $\bar{V}_2$ , and the equality is again satisfied by  $\bar{V}_2 = v$ .

Here, we sketch the proof in the first case, the second case being analogous. Let us suppose that at a given point  $x_0 \in S_1$  the potential satisfies  $V(x_0) = \bar{V}_1 > v$ , and consider two intervals  $\omega$  and  $\chi$  of the same length  $\epsilon$ ,  $\omega$  lying in  $S_2$  and bordered by a domain wall, and  $\chi$  lying in  $S_1$

and containing  $x_0$ . The chemical potentials are fixed; thus, the functional form of the density functions does not depend on the positions of the domain walls. We now replace in  $\omega$  the first species with the second one, and in  $\chi$  the second species with the first one, using again TF density functions. Taking into account condition (54), we find that the difference between the energy of the final and the initial configurations is

$$\delta\mathcal{E} = \epsilon \frac{(\mu_1 - \bar{V}_1)^2}{2} \left[ 1 - \left( \beta \frac{\mu_2 - \bar{V}_1}{\mu_1 - \bar{V}_1} \right)^2 \right] + \mathcal{O}(\epsilon^2). \quad (91)$$

For sufficiently small  $\epsilon$ , the final configuration is energetically favored with respect to the initial one, if condition (89) applies. We finally note that, unlike in (83)–(85), the conditions (89) and (90) are independent of the value of  $v$ . Even in this case, since usually  $\beta^2 = U_{11}/U_{22} \simeq 1$ , conditions (89) and (90) preclude any non-maximal stable configuration from being the ground state.

### 4.3. Outlook

Let us give a brief summary of the results obtained and the strategy adopted in this paper. The main objective is to determine the stationary (separated) configurations of the mixture. Let us focus on the case in which the particle numbers  $N_1$  and  $N_2$  are fixed, since this case is complicated by the normalization conditions on the density profiles. Let us suppose that equation (57),  $\varphi(x) = f$ , has at most  $n$  solutions, and let us fix the number of domain walls  $m \leq n$ . Condition (54), together with normalization, yields a set of three equations:

$$\begin{aligned} \mu_1 - \mu_2 &= V_1(x) - V_2(x) \equiv \varphi(x), \\ N_1 &= \mu_1 |S_1^{(m)}| - \int_{S_1^{(m)}} dx V_1(x), \\ N_2 &= \mu_2 |S_2^{(m)}| - \int_{S_2^{(m)}} dx V_2(x), \end{aligned} \quad (92)$$

where  $S_k^{(m)}$  are the supports of the density profiles. The solutions of equations (92) completely determine the stationary configurations that can be conveniently found in this way, rather than by directly minimizing the energy functional. Once the stationary configurations are identified for different numbers of domain walls, it is possible to compute their energy and determine the ground state.

In the case of proportional trapping potentials, it emerges that configurations with a maximal number of domain walls are usually energetically favored, and the less self-interacting species tends to occupy the minima of the potential. In this case, condition  $\varphi(R_j) = f$  specializes to  $V_1(R_j) \equiv V(R_j) = v$ . Thus, a convenient procedure to find the ground-state configuration would be (refer to figure 2 for concreteness) to choose an initial small value of  $v$  and start with the maximal number of domain walls satisfying  $V(R_j) = v$ ; then adjust  $v$  until the normalization conditions are satisfied. If normalizations cannot be fulfilled,  $v$  must be increased (so that the number of domain walls is reduced) and the procedure should be repeated, until a solution is found.

The approach and procedure are self-consistent and must (physically) stop and yield a solution when there are at least two domain walls (in the present working hypotheses—regularity and confinement (14)—for the potentials). The method is applicable for general regular potentials and its relative simplicity is one of the main results of this paper.

## 5. Conclusion

We have studied the Thomas–Fermi equations for a system of two Bose–Einstein condensates confined in generic potentials. We have emphasized the role of the limiting value

$U_{12} = \sqrt{U_{11}U_{22}}$  in determining if the ground state of the system is a mixed configuration or a separated one by assuming that the external potentials are regular. We determined a set of conditions to be satisfied by locally stable separated configurations. We then looked for the ground state among the possible locally stable configurations and found that those with a maximal numbers of domain walls are usually energetically favorite. The results presented in this paper enable us to find the ground state of binary mixtures in multi-well potentials, given either the numbers of particles or the chemical potentials.

It would be interesting to analyze the changes that a correction to the TF approximation, including the kinetic energies, would introduce in such a picture. If the numbers of particles are sufficiently high, the TF approximation is very accurate. Nonetheless, TF density profiles correspond to diverging kinetic energy, due in particular to the discontinuities at the domain walls. The kinetic parts intervene by regularizing the TF solutions, at the expense of an increase in the potential energy, especially in a neighborhood of a domain wall. This could lead to an inversion in the energetic diagram, in which configurations with few domain walls could become energetically favorite with respect to maximal stable configurations. This inversion has already been numerically studied in the simple case of a harmonic potential [2], but the tools introduced in this paper uncover the possibility of extending this kind of analysis to generic multi-well potentials, such as arrays of optical traps, which are now within experimental reach.

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