Ground state geometry of binary condensates in axisymmetric traps

S Gautam and D Angom

Physical Research Laboratory, Navarangpura, Ahmedabad, 380 009, India

Received 1 December 2009, in final form 15 March 2010
Published 15 April 2010
Online at stacks.iop.org/JPhysB/43/095302

Abstract

We show that the ground state interface geometry of binary condensates in the phase-separated regime undergoes a smooth transition from planar to ellipsoidal to cylindrical geometry. This occurs for the condensates with repulsive interactions as the trapping potential is changed from prolate to oblate. The correct ground state geometry emerges when the interface energy is included in the energy minimization, whereas energy minimization based on the Thomas–Fermi approximation gives incorrect geometry. The planar and cylindrical interface geometries have less interface area and minimize the interface energy. These are the preferred ground states in the cigar- and pan-cake-shaped trap configurations.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The two-species Bose–Einstein condensate (TBEC), consisting of two different hyperfine spin states of \(^{87}\)Rb, was first observed by Myatt et al [1]. Since then, TBECs of different atomic species \((^{41}\)K and \(^{87}\)Rb) [2] and of different isotopes of the same atomic species [3] have been experimentally realized. This has led to several experimental and theoretical investigations on different aspects of TBECs. The remarkable feature of TBECs, which is absent in a single-component Bose–Einstein condensate (BEC), is the phenomenon of phase separation. In the Thomas–Fermi approximation (TFA), the phase separation occurs when all the inter-atomic interactions are repulsive and the inter-species repulsion exceeds the geometric mean of the intra-species repulsive interactions.

Depending upon the properties of the condensates and trapping potential parameters, the ground state of TBECs assumes a configuration which minimizes the total energy. The structure of the ground state plays an important role in dynamical phenomena such as Rayleigh–Taylor [4, 5] instability, Kelvin–Helmholtz instability [6], modulational instability [7–9], pattern formation at the interface [10], etc. It was recently demonstrated that quantum Rayleigh Taylor instability can be observed in a very controlled way with TBECs in cigar-shaped traps [4].

In the phase-separated regime, the interface energy of the two component species defines the geometry of the ground state. In a previous work, the ground state geometry of TBECs was examined within the TFA [11], i.e. without the interface energy. In later works, [12–14] the contribution from the interface energy was incorporated. From these it is observed that the analytic approximations for interface energy are not sufficient enough to explain the experimental results of strongly segregated ground states [3]. A recent work [15] reported a more accurate determination of the interface energy. It explains the stationary state geometry of the strongly segregated TBECs more precisely.

In this paper, we provide a semi-analytic scheme to determine the stationary state structure of TBEC in axisymmetric traps. For this, we follow the ansatz adopted in [16], i.e. to minimize the total energy of TBEC with fixed number of particles of each species in TFA. We find that depending on trapping potential parameters, a TBEC can assume three distinct geometries in axisymmetric traps: planar, ellipsoidal and cylindrical. However, we observe that without the interface energy correction, the ellipsoidal geometry is the ground state. This is not surprising as the density depends only on the trapping potential in the TFA, and the ellipsoidal geometry matches the equipotential surfaces of the potential. The planar and the cylindrical interface geometries emerge as the ground state structures of the cigar-shaped and the pan-cake-shaped trapping potentials respectively, when the interface energy is incorporated, the reason being that interface energy depends upon the area and density distribution at the interface. For the cigar- and pan-cake-shaped traps, the area of the interface is significantly lower for the planar and the cylindrical geometries respectively. Hence, these geometries have less interface energy and minimize the total energy.
To validate the results of our semi-analytic approach, we numerically solve the coupled pair of Gross–Pitaevskii (GP) equations which describes the TBEC. The numerical results are in good agreement with the semi-analytic ones.

The paper is organized as follows: in section 2 of the manuscript, we elaborate on the semi-analytic scheme to determine the parameters of the ground state for each of the three geometries using the TFA. In section 3, we examine the role of interface energy in determining the ground state structure of the TBEC.

2. TBEC in axisymmetric traps

We consider a TBEC in axisymmetric trapping potentials

\[ V_i(r, z) = \frac{m_i}{2} (\alpha_i^2 r^2 + \lambda_i^2 z^2), \]

where \( i = 1, 2 \) is the species index, and \( \alpha_i \) and \( \lambda_i \) are the anisotropy parameters. In the mean field approximation, the stationary state solution of the binary condensate is described by a set of coupled GP equations

\[
\begin{bmatrix}
-\hbar^2 \nabla^2 + V_i(r, z) + \sum_{j=1}^2 U_{ij}|\psi_j(r, z)|^2 - \mu_i
\end{bmatrix} \psi_i(r, z) = 0.
\]

Here, \( i \) and \( j = 3 - i \) are species indices, \( U_{ij} = 4\pi\hbar^2 a_{ij}/m_i \) with \( m_i \) as mass and \( a_{ij} \) as s-wave scattering length is the intra-species interaction, \( U_{ii} = 2\pi\hbar^2 a_{ii}/m_i \) with \( m_{ij} = m_i m_j / (m_i + m_j) \) as reduced mass and \( a_{ij} \) as inter-species scattering length is the inter-species interaction term and \( \mu_i \) is the chemical potential of the \( i \)th species.

When the number of atoms is large, the TFA is applicable to obtain the stationary state solutions of equation (2). In this limit, the kinetic energy is neglected in comparison to interaction energy. We consider the interaction parameter \( U_{12} > \sqrt{U_{11}U_{22}} \) such that the two components are phase separated, the two components occupy different regions of the trapping potentials. Neglecting the overlap between the species, stationary state solutions within the TFA are

\[ |\psi_i(r, z)|^2 = \frac{\mu_i - V_i(r, z)}{U_{ii}}, \]

where \( \mu_i \) is fixed by the number of atoms of the corresponding species.

The total energy of the TBEC in the phase-separated regime is

\[ E = \int dV \left[ V_1(r, z)|\psi_1(r, z)|^2 + V_2(r, z)|\psi_2(r, z)|^2 + \frac{1}{2} U_{11}|\psi_1(r, z)|^4 + \frac{1}{2} U_{22}|\psi_2(r, z)|^4 \right]. \]

Depending upon the anisotropy parameters, the TBEC can have three distinct spatial distributions in axisymmetric traps. The distinguishing feature of these structures is the geometry of the interface, which can be planar, cylindrical or ellipsoidal. The smooth transition of interface geometry, for the TBEC of \(^{85}\text{Rb} - ^{87}\text{Rb}\) mixture, from planar to ellipsoidal and finally to cylindrical is shown in figure 1. These features are most prominent when the TBEC is strongly segregated. For the detailed examination of our scheme, we choose \(^{85}\text{Rb} - ^{87}\text{Rb}\) experiments of Papp et al [3], where two of the geometries planar and ellipsoidal were observed.

2.1. Planar interface

It has been observed experimentally [3] in cigar-shaped traps \((\lambda_i \ll \alpha_i)\) that the TBEC assumes a sandwich structure with planar interface between the two species. In this structure the phase separation occurs along the axial direction, and the strongly interacting component sandwiches the weakly interacting one. There are two realizations of this: coincident and shifted trapping potentials.

2.1.1. Coincident trap centres. An idealized choice of \( V_i \) is with coincident centres. If \( z = \pm L_1 \) are the locations of the planes separating the two components, and \( L_2 \) is the axial extent of the binary condensate, then the problem of determining the structure of the TBEC is equivalent to calculating \( L_1 \). If \( N_i \) and \( R_i \) are the number of atoms and radial size of the \( i \)th species respectively, then

\[ N_i = 2\pi \int_0^{R_i} r \, dr \int_{-L_i}^{L_i} dz |\psi_i(r, z)|^2. \]

From equation (3), we get

\[ N_1 = 2\pi \left( \frac{\omega^2 L_1^3 m_1 \lambda_1^4}{20 U_{11} \alpha_1^2} + \frac{L_1 \lambda_1^2 \mu_1}{3 U_{11} \alpha_1^2} + \frac{L_1 \lambda_1^2}{\omega^2 m_1 U_{11} \alpha_1^2} \right), \]

\[ N_2 = 4\pi \left[ \frac{4\sqrt{2} \mu_2 \lambda_2}{50 \omega^2 m_2 U_{22} \alpha_2^2} + \frac{L_1}{120 U_{22} \alpha_2^2} \left( \frac{5\omega^2 L_1^3 m_2 \lambda_2^4}{\lambda_2 L_1} + 20 L_1^2 \lambda_2^2 \mu_2 \right) - \frac{8\omega^2 m_2 (L_1 \lambda_2^3 \lambda_1^{5/2})}{\lambda_2 L_1} + \frac{60 \mu_2^2}{\omega^2 m_2} \right]. \]
Similarly, the total energy in equation (4) is

\[
E = \frac{4\pi}{16800\omega^2 m_2 U_{22} \alpha_2^2} \left[ -21\alpha^6 L_1^2 m_2^3 \lambda_2^5 + 16\alpha^6 L_1^2 m_2^3 \lambda_1^5 
+ 112\alpha^4 L_1^2 m_2^3 \lambda_2^5 \mu_2 - 112\alpha^4 L_1^2 m_2^3 \lambda_2^5 \mu_2 + 140\alpha^2 L_1^2 m_2^3 \lambda_2^5 \mu_2 
\right] 
\times \frac{\mu_2}{\omega^3 \lambda_2^3 m_2^2}
\]

\[
+ 2\pi \left( \frac{\omega^2 L_1^2 m_2 \lambda_1^2}{168 \omega^2 \alpha_2^2} + \frac{L_1^2 \lambda_2^2 \mu_2}{6 \omega^2 \alpha_2^2} + \frac{2 L_1^2 \mu_2}{3 \omega^2 m_2 \alpha_2^2} \right). 
\] (7)

Here, \(L_1\) is determined through the variational minimization of \(E\) with \(L_1\) as the variational parameter and constraints that \(\mu_1\) and \(\mu_2\) satisfy equation (6) for fixed \(\mu_1\). In the constraint equations, we invert the expression of \(N_1\) and obtain \(\mu_1\) as a function of \(L_1\). However, inverting \(\mu_2\) to calculate \(\mu_2\) is nontrivial and hence we implement the minimization numerically.

As mentioned earlier, we consider the TBEC of \(^{85}\)Rb–\(^{87}\)Rb with \(N_1 = 50,000\). For this TBEC, scattering lengths \(a_1 = 5\lambda_1\), \(a_2 = 99\lambda_1\), and \(a_12 = 214\lambda_1\) are taken from the experimental results of Wieman and collaborators [3]. Likewise, the anisotropy parameters and trap frequency are \(\alpha_1 = 1\), \(\lambda_1 = 2.9/130\), \(\lambda_2 = 2.6/130\) and \(\omega = 130\) Hz respectively. From here on, this choice of parameters is referred to as set \(a\). For these parameters, the minima of \(E\) occurs at 32.3\(\mu_0\). Here, the unit of length \(\mu_0\) referred to as the oscillator length is \(\sqrt{\hbar/m_2 \omega}\). To corroborate the results we solve equation (2) numerically and find that the semi-analytic results are in good agreement with the value of 33.8\(\mu_0\) obtained from the numerical solution. For this we employ the split-step Crank–Nicholson method [17] implemented for binary condensates. Based on the numerical results, the profile of \(\psi^2\) for \(^{85}\)Rb and \(^{87}\)Rb is shown in figure 1.

2.1.2. Separated trap centres. In the experimental realizations, the gravitational potential of Earth and tilts in the external field configurations tend to separate the minima of the effective potentials. Normally in the cigar-shaped traps, the tilt angle is small and separation is effectively along the axial direction. The potentials with separation \(z_0\) are

\[
V_1(r, z) = \frac{m_1 \alpha_1^2}{2} \left( \alpha_1^2 r^2 + \lambda_1^2 z^2 \right),
\]

\[
V_2(r, z) = \frac{m_2 \alpha_2^2}{2} \left( \alpha_2^2 r^2 + \lambda_2^2 (z - z_0)^2 \right). 
\] (8)

Due to the loss of axial symmetry, \(z = -l_1\) and \(z = l_1\) are the two planes separating the two components. These, \(l_1\) and \(l_1\), are the parameters to minimize \(E\). Like in the previous subsection, \(N_1, N_2\) and \(E\) can be evaluated, and the expressions are presented in the appendix. For the parameter set \(a\) and \(z_0 = 3.4\ \mu\), the minima of \(E\) occurs when \(l_1\) and \(L_1\) are 39.5\(\mu_0\) and 26.0\(\mu_0\) respectively. The overall trend of \(E\) as a function of the variation parameters is shown in figure 2. It is evident from the figure, for the chosen set of parameters, that the energy minima is not strongly localized. In other words, around the energy minima there is little variation of \(E\) as a function of \(l_1\) and \(L_1\). Noticeable features of the iso-energy curves, contours in figure 2, are the ellipse shape and orientation. These indicate the trend of how change in one parameter \(l_1\) (\(L_1\)) is balanced with a change in the other parameter \(L_1\) (\(l_1\)) to maintain constancy of energy. The variations along the iso-energy curves can perhaps occur as temporal variations when the TBEC is excited or the ground state is perturbed.

2.2. Ellipsoidal interface

As the anisotropy parameter \(\lambda\) is increased beyond a critical value \(\lambda_c\), the interface geometry changes from planer to ellipsoidal where one species envelopes the other. This is the preferred interface geometry for the phase-separated TBEC in axisymmetric traps without interface energy. Consider trapping potentials with coincident centres. If \(R_1\) and \(L_1\) are equatorial (along radial direction) and polar (along axial direction) radii of the \(i\)th species respectively, then

\[
N_i = 2\pi \int_{0}^{R_i} r \, dr \int_{-L_i}^{L_i} dz |\psi_i(r, z)|^2.
\] (9)

From equations (3) and (4), we get

\[
N_1 = -2\pi R_1 \alpha_1 \left( 3 \omega^2 m_1 R_1^2 \alpha_1^2 - 10 R_1^2 \mu_1 \right), 
\]

\[
N_2 = 2\pi \frac{R_2}{15 \mu_2 \alpha_2} \left( \omega^2 m_2 R_2^2 \alpha_2^2 (2 \alpha_2^2 \lambda_1^2 + 3 \alpha_1^2 \lambda_2^2) 
- 10 R_2^2 \alpha_1^2 \lambda_1^2 \mu_2 + \frac{8 \sqrt{2} \lambda_1 \mu_2}{\lambda_2 \lambda_1^2 \omega^2 m_2} \right). 
\] (11)

\[
E = \frac{\pi}{210 \omega^2 m_2 U_{11} \alpha_2^2 \lambda_1^2 \lambda_2^2} \left( -15 \omega^2 m_2^2 m_3 R_1^2 U_{22} \alpha_2^2 \lambda_1^2 \lambda_2^2 
+ \omega^2 m_2^2 R_1^2 U_{11} \alpha_1^2 \alpha_2^2 (8 \alpha_2^2 \lambda_1^2 + 4 \alpha_2^2 \lambda_1^2 \alpha_1^2 \lambda_2^2 + 3 \alpha_1^2 \lambda_2^2) 
+ 160 \sqrt{2} U_{11} \lambda_1^2 \mu_2 \alpha_1^2 \lambda_1^3 \lambda_2^2 (U_{22} \mu_2^2 - U_{11} \mu_2^2) \right). 
\] (12)
In the TFA, the profile of density \(|\psi_i(r, z)|^2\) has the same ellipticity

\[
e = \begin{cases} \frac{\alpha_i^2 - \lambda_i^2}{\alpha_i^2} & \text{if } \lambda_i < 1 \text{ (prolate)}, \\ \frac{\lambda_i^2 - \alpha_i^2}{\lambda_i^2} & \text{if } \lambda_i > 1 \text{ (oblate)}, \end{cases} \tag{13}
\]

as that of the trapping potential. This is evident from the expression of density with the TFA given in equation (3), where only the trapping potential \(V_i(r, z)\) has spatial dependence. The value of \(R_i\) depends on \(\mu_2\) and reduces the variation parameter to only \(R_1\). From the ellipticity of the trapping potential, the axial radius of the ellipsoidal interface \(L_i\) is \(\alpha_i R_i / \lambda_i\). The energy \(E\) is then minimized numerically to find the equilibrium geometry of the phase-separated TBEC. To examine the scheme, consider the \(^{85}\text{Rb} - ^{87}\text{Rb}\) mixture with the parameter set \(a\) and coincident trapping potentials, but take \(\lambda_i\) as 1.5. Then the equilibrium geometry is ellipsoidal with an equatorial radius \(R_i\) of 3.72\(\omega_{\text{osc}}\). This is in very good agreement with value 3.75\(\omega_{\text{osc}}\) obtained from the numerical solution of GP equations. The pseudo colour-coded \(|\psi_i|\) of \(^{85}\text{Rb}\) and \(^{87}\text{Rb}\), numerically computed, of the ellipsoidal interface are shown in figures 1(b)–(e). It is to be noted that in the images, the interface is prolate when \(\lambda_i < 1\) and oblate when \(\lambda_i > 1\). These interface geometries are similar to the topologies of the equipotential surfaces of the trapping potential. A highly symmetric case is when \(\lambda_i\) is unity; the interface geometry is then spherical in shape.

2.3. Cylindrical interface

On further increase of \(\lambda_i\) beyond another critical value \(\lambda_{i_b}\), the equilibrium interface geometry is like a cylinder, where the axis of the interface coincides with the polar axis of the trapping potentials. It occurs in the oblate condensates, and here the phase separation is along the radial direction. Here the phase separation is along radial direction and is analogous to planar interface in cigar-shaped condensates. The reasons for the emergence of the cylindrical geometry as the ground state geometry will become clear in the following section where we discuss the role of interface energy. If \(\rho_i\) is the radius of the interface cylinder, then in the TFA

\[
N_1 = -\frac{4\pi(\alpha_i^2 \rho_i^2 m_1 \alpha_i^2 - 2 \mu_1)^2}{15 \omega m_1 U_{11} \lambda_i \alpha_i^2} - \frac{16\pi \sqrt{2} \mu_i^{5/2}}{15 U_{11} \lambda_i \alpha_i^2 (m_1 \omega^2)^{3/2}},
\]

\[
N_2 = \frac{4\pi(\rho_i^2 \rho_i^2 m_2 \alpha_i^2 - 2 \mu_2)^2}{15 \omega m_2 U_{22} \lambda_i \alpha_i^2},
\]

\[
E = -\frac{4\pi}{15 U_{11}} \left( -\frac{20 \sqrt{2} \mu_i^{7/2}}{7 \lambda_i \alpha_i^2 (m_1 \omega^2)^{3/2}} + \frac{(\rho_i^2 \rho_i^2 m_1 \alpha_i^2 - 2 \mu_1)^2}{7 \omega m_1 \lambda_i \alpha_i^2} \right) \left( \omega^2 \rho_i^2 m_1 \alpha_i^2 + 5 \mu_1 \right) \sqrt{-\rho_i^2 \alpha_i^2 + \frac{2 \mu_1}{\omega m_1}} \right) \tag{14}
\]

The above set of equations define the stationary state of the TBEC in the oblate-shaped condensates. Like in the planar geometry, \(\rho_i\) is the parameter of variation. To verify the scheme, we consider a pan-cake-shaped \((\lambda_i \gg \alpha_i)\) TBEC of \(^{85}\text{Rb} - ^{87}\text{Rb}\) mixture in coincident traps with \(\lambda_i\) as 50.0 and the parameter set \(a\). Then from our scheme, the equilibrium state has cylindrical interface of radius 5.84\(\omega_{\text{osc}}\). The value from the numerical solution of the GP equation is 5.89\(\omega_{\text{osc}}\).

The two results are in very good agreement and validate our minimization scheme. The contour plots, showing the absolute value of wavefunctions of \(^{85}\text{Rb}\) and \(^{87}\text{Rb}\), obtained by numerically solving equation (2) are shown in figure 1(f). Experimentally, the cylindrical geometry has not been observed in TBECs due to the fact that the \(\lambda_i\) of the trapping potentials were not large enough.

3. Role of the interface energy

In the TFA calculations discussed so far, as mentioned earlier, the interface energy is neglected. Accordingly, the variational schemes we have adopted incorporate appropriate interface geometries. However, a general minimization by considering all the possible interface geometries favors the ellipsoidal interface as the equilibrium configuration. For example, though the cylindrical interface for \(\lambda_i = 50.0\) reproduces the numerical results for the TBEC of \(^{85}\text{Rb} - ^{87}\text{Rb}\) with the parameter set \(a\), the minimization with ellipsoidal interface has lower \(E\). This is evident from the values of \(E\), calculated over a wide range of \(\lambda_i\) for the three interface geometries, shown in figure 3.
As discussed in [15], the planer interface observed in experiments [3] emerges as the equilibrium geometry when the interface energy is considered. When $\theta_{mic}$ is much larger than the interface thickness, the total excess energy arising from the finite interface tension [15] is

$$\Omega_A = \frac{\sqrt{2m_1}}{4\pi\hbar a_{11}} F(\xi_2/\xi_1, K) \int d\mathbf{r} [\mu_1 - V(\mathbf{r})]^{3/2}. \quad (15)$$

Here $\xi_i$ are the coherence lengths and $K, \xi_2/\xi_1$ and $F(\xi_2/\xi_1, K)$ are defined as

$$K = \frac{(m_1 + m_2)a_{12}}{2\sqrt{m_1 m_2 a_{11} a_{22}}}, \quad \frac{\xi_2}{\xi_1} = \left(\frac{m_1 a_{11}}{m_2 a_{22}}\right)^{1/4},$$

$$F(\xi_2/\xi_1, K) = \frac{\sqrt{2}}{3} \left(1 + \frac{\xi_2}{\xi_1}\right) - \frac{0.514\sqrt{\xi_2/\xi_1}}{K^{1/4}} + \frac{0.055}{K^{3/4}} + \frac{0.067}{K^{5/4}} + \cdots,$$

where the integration is over the interface surface area $A$. The above expression is valid provided $K \gg 1.5$ and $\xi_2/\xi_1 \ll 1$. In the present work, we consider TBECs in the strongly segregated regime with $\xi_2/\xi_1 < 1$, and hence the interface energy in equation (15) is applicable. Furthermore, the interpenetration depth is proportional to $\sqrt{\xi_2/\xi_1}/K^{1/4}$ and approaches zero in the limit $1/K \to 0$. In this limit, there is no overlap, and the TFA solution is an excellent approximation. The equilibrium geometry is then the one which minimizes the total energy: sum of TFA energy and $\Omega_A$.

A precise determination of $\Omega_A$ is, therefore, essential to obtain correct geometry of the phase-separated TBEC. In relative comparison, we find that the geometry which has the least interface area is also the one with the minimum interface energy. The interface area in planar and cylindrical geometries are

$$A = \left\{\begin{array}{ll}
2\pi \frac{2\mu_1 - \lambda_1^2 L_1^2}{\alpha_1} & \lambda \ll 1 \quad (\text{planar}), \\
4\pi \rho \sqrt{2\mu_1 - \alpha_1^2 \rho^2} & \lambda \gg 1 \quad (\text{cylindrical}).
\end{array}\right. \quad (16)$$

Similarly, for the prolate and oblate geometries the interface areas are

$$A = \left\{\begin{array}{ll}
2\pi R_1^2 + 2\pi R_2^2 \frac{\alpha_1}{\epsilon} \sin^{-1} e & \rho \ll 1 \quad \text{prolate}, \\
2\pi R_1^2 + \frac{\pi}{e} \frac{\alpha_1 R_1}{\lambda_1} & \rho \gg 1 \quad \text{oblate}. \quad (17)
\end{array}\right.$$

Here the ellipticities $e$ are as defined earlier in equation (13). The interface areas in the three geometries for the TBEC of $^{85}$Rb–$^{87}$Rb mixture, for three geometries: planar (brown curve), ellipsoidal (black curve) and cylindrical (orange curve). The inset plot shows the interface energy.

Figure 4. Plots showing the interface areas as the functions of $\lambda$, in the TBEC of the $^{85}$Rb–$^{87}$Rb mixture, for three geometries: planar (brown curve), ellipsoidal (black curve) and cylindrical (orange curve). The inset plot shows the interface energy.

more crucial than the interface area to determine the ground state geometry.

In the following subsections, we examine the impact of $\Omega_A$ in two domains: prolate-shaped potentials ($\lambda_i < 1$) and oblate-shaped potentials ($\lambda_i > 1$). For higher symmetry and simplified analysis we choose $\lambda_1 = \lambda_2 = \lambda$.

3.1. Prolate trapping potentials

In the $\lambda < 1$ domain, at low values of $\lambda$, the ellipsoidal geometry has higher ground state energy than the planar geometry. As $\lambda$ is increased, keeping the other parameters fixed, the ground state energies of both the geometries increase; however, the planar geometry has higher rate of increase. At $\lambda_{\alpha}$, which is close to 1, the energies of the two geometries are equal. Beyond this critical value, the energy of the ellipsoidal geometry is lower and is the ground state geometry. This can be understood from the rate at which the interface areas of these two geometries change as $\lambda$ is increased. With the increase in $\lambda$, the interface area of planar geometry increases while that of ellipsoidal geometry decreases. Furthermore, the average rate of change in ellipsoidal geometry is higher than that of planar geometry, which is evident from figure 4. Hence, the planar geometry is the ground state geometry due to the much smaller interface area and consequently lower interface energy correction for $\lambda \ll 1$. On the other hand, for $1 > \lambda > \lambda_{\alpha}$, ellipsoidal geometry emerges as the ground state geometry due to the lower interface energy correction arising from a smaller interface area.

For the $^{85}$Rb–$^{87}$Rb mixture with the parameter set $a$, the total energy $E$, obtained by incorporating $\Omega_A$ in the semi-analytic scheme developed in previous section, and interface energy $\Omega_A$ as functions of $\lambda$ for the two geometries are respectively shown in figures 3 and 4 (inset plot). As the value of $\lambda_{\alpha}$ depends on the parameters of the system, we examine the variation in $\lambda_{\alpha}$ as a function of the ratio $N_2/N_1$. For this, we fix $N_1$ and vary $N_2$, then calculate $\lambda_{\alpha}$ as a function $N_2/N_1$. When $N_2$ is decreased $\lambda_{\alpha}$ increases initially and then decreases. This is shown in figure 5.
respectively) and ratio of population $N_2/N_1$ in the TBEC of the $^{85}\text{Rb} -^{87}\text{Rb}$ mixture. Inset plots show the variation in energy of two lowest energy structures with $\lambda$ for oblate trapping potentials with interface energy correction. Black and brown curves correspond to ellipsoidal and cylindrical geometries respectively, whereas orange curve represents $E$ as a function of $\lambda$. Each pair of curves corresponds to different $N_1$ but same $N_1$. The uppermost pair is for $N_1 = N_2 = 50\,000$. The next lower pair of curves has $N_2 = 46\,000$, $42\,000$, and so on.

**Figure 5.** Ground state geometry as a function of $\lambda_s$ ($\lambda_s$ and $\lambda_0$ for planar–ellipsoidal and ellipsoidal–cylindrical transition respectively) and ratio of population $N_2/N_1$ in the TBEC of the $^{85}\text{Rb} -^{87}\text{Rb}$ mixture. Inset plots show the variation in energy of two lowest energy structures with $\lambda$ for oblate trapping potentials with interface energy correction. Black and brown curves correspond to ellipsoidal and cylindrical geometries respectively, whereas orange curve represents $E$ as a function of $\lambda$. Each pair of curves corresponds to different $N_1$ but same $N_1$. The uppermost pair is for $N_1 = N_2 = 50\,000$. The next lower pair of curves has $N_2 = 46\,000$, $42\,000$, and so on.

**Figure 6.** False colour-coded cutaway view of $|\psi_i(r, z)|$ for the cylindrical interface of the $^{85}\text{Rb} -^{87}\text{Rb}$ mixture. Inset plots show the variation in energy of two lowest energy structures with $\lambda$ for oblate trapping potentials with interface energy correction. Black and brown curves correspond to ellipsoidal and cylindrical geometries respectively, whereas orange curve represents $E$ as a function of $\lambda$. Each pair of curves corresponds to different $N_1$ but same $N_1$. The uppermost pair is for $N_1 = N_2 = 50\,000$. The next lower pair of curves has $N_2 = 46\,000$, $42\,000$, and so on.

### 4. Conclusions

There are three distinct interface geometries of the ground state of TBECs in the phase-separated regime. We have developed a semi-analytic scheme to determine the stationary state parameters for each of these and demonstrate the validity of the scheme by comparing semi-analytic results with the numerical ones. We find in the TFA, when the interface energy is neglected, the ellipsoidal geometry has the lowest energy for all values of $\lambda$. Hence, it is the preferred ground state structure. In this structure, one species envelopes the other, and interface geometry and overall shape of the TBEC is ellipsoidal. To explain the experimentally realized stationary state structures of TBECs, we incorporate the interface energy in our semi-analytic scheme. We find that minimizing total energy, sum of TFA energy and $\Omega_A$, gives the right interface geometry. Then in our semi-analytic scheme the ellipsoidal geometry no longer has the lowest energy for all values of $\lambda$. For cigar-shaped traps ($\lambda \ll 1$), the structure with the planar interface is the ground state geometry, while for pancake-shaped traps ($\lambda \gg 1$) the cylindrical interface is the ground state geometry. For the values of $\lambda$ close to unity, ellipsoidal structure is the ground state geometry.

**Appendix**

In the case of planar interface between the two species trapped in potentials with separated minima, the expressions for $N_1$, $N_2$ and $E$ are

$$N_1 = \frac{\pi}{60U_{11}\alpha_1^2} \left[ 3\omega^2(l_1^5 + L_1^5) m_1 \lambda_1^5 + 20(l_1^3 + L_1^3) \lambda_1^3 \frac{60(l_1 + L_1) \mu_1}{\omega^2 m_1^3} \right], \quad (A.1)$$

$$N_2 = \frac{1}{3\lambda_2 U_{22}} \pi \left[ 8\sqrt{2} \mu_2 \left( \frac{\mu_2}{\omega m_2^3} \right)^{3/2} + \frac{1}{20\omega^3 m_2^2 \alpha_2^2} \right. \times (5\omega^4 l_1^5 m_2^3 \lambda_2^5 - \omega^2 l_1^3 m_2^1 \lambda_2^1 (15 \omega \lambda_2 + 8 \lambda_1 \lambda_2 - 10 \lambda_2 \mu_2 \right) + 20 \mu_2 \lambda_2 \times (\omega^2 m_2^3 \lambda_2^3 - 3 \mu_2) \mu_2 + 60 \lambda_2 l_1 (\omega^2 m_2^3 \lambda_2^3 - 2 \mu_2) \mu_2 + 10 \mu_2 \lambda_2 \left. \times \left[ \frac{1}{\lambda_2 U_{22}} \pi \left[ -8 \sqrt{2} \mu_2 \left( \frac{\mu_2}{\omega m_2^3} \right)^{3/2} + \frac{1}{20\omega^3 m_2^2 \alpha_2^2} \right] \times (-5\omega^4 L_1^5 m_2^3 \lambda_2^5 + \omega^2 L_1^3 m_2^1 \lambda_2^1 (-15 \omega \lambda_2 + 8 \lambda_1 \lambda_2) \right] \right]$$
\[ E = \frac{1}{60 U_{22}} \left[ \frac{160\sqrt{2} \mu_2}{7 \omega^2 m_2 a_2^2} - \frac{1}{14} \omega^2 m_2 a_2^2 \right] \times \left[ 21\omega^6 L_1^3 m_2^3 \lambda_2^3 \left( \frac{35 \omega^2 m_2 \lambda_2^2 - 4 \omega^2 m_2 \lambda_2^2}{2 \mu_2} \right) \right] + \frac{\pi}{168 U_{11} a_1} \left( \omega^6 (L_1^3 + L_1^3) m_1^3 \lambda_1^6 - 28 (L_1^3 + L_1^3) m_1^3 \lambda_1^6 \right) + \frac{112 (L_1 + L_1) m_1^3}{\omega^2 m_1} \right). \] (A.3)

These equations reduce to those for coincident centres on substituting \( L_1 = L_1 \) and \( \omega_0 = 0 \).

References

[1] Myatt C J, Burt E A, Ghest R W, Cornell E A and Wieman C E 1997 Phys. Rev. Lett. 78 586
[2] Modugno G, Modugno M, Riboli F, Roati G and Inguscio M 2002 Phys. Rev. Lett. 89 190404
[3] Papp S B, Pino J M and Wieman C E 2008 Phys. Rev. Lett. 101 040402
[4] Gautam S and Angom D 2009 arXiv:0908.4336v3
[5] Sasaki K, Suzuki N, Akamatsu D and Saito H 2009 Phys. Rev. A 80 063611
[6] Takeuchi H, Suzuki N, Kasamatsu K, Saito H and Tsubota M 2010 Phys. Rev. B 81 094517
[7] Kasamatsu K and Tsubota M 2004 Phys. Rev. Lett. 93 100402
[8] Raju T S, Panigrahi P K and Porsezian K 2005 Phys. Rev. A 71 035601
[9] Ronen S, Bohn J L, Halmo I E and Edwards M 2008 Phys. Rev. A 78 053613
[10] Saito H, Kawaguchi Y and Ueda M 2009 Phys. Rev. Lett. 102 230403
[11] Ho T-L and Shenoy V B 1996 Phys. Rev. Lett. 77 3276
[12] Timmermans E 1998 Phys. Rev. Lett. 81 5718
[13] Ao P and Chui S T 1998 Phys. Rev. A 58 4836
[14] Barankov R A 2002 Phys. Rev. A 66 013612
[15] Van Schaeybroeck B 2008 Phys. Rev. A 78 023624
[16] Trippenbach M, Goral K, Rzazewski K, Malomed B and Band Y B 2000 J. Phys. B: At. Mol. Opt. Phys. 33 4017
[17] Muruganandam P and Adhikari S K 2009 Comput. Phys. Commun. 180 1888