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LETTER TO THE EDITOR

Amplification of trap centres position difference in mixtures of Bose–Einstein condensates

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Online at stacks.iop.org/JPhysCM/14/L77**Abstract**

We show by analytic calculation and numerical simulation that the effect of trap displacements are amplified in mixtures of Bose–Einstein condensates, consistent with experimental observations. We also investigate the relative stability of inner and outer vortex states as the minima of the trapping potentials are displaced along the axis of rotation.

Mixtures of Bose–Einstein condensates (BEC) in traps have recently received considerable interest [1, 2]. Hall and co-workers [1] studied a condensate consisting of simultaneously trapped atoms of ⁸⁷Rb in two different hyperfine spin states $|1\rangle = |F = 1, m_f = -1\rangle$ and $|2\rangle = |2, 1\rangle$ with trapping potentials V_1, V_2 . The scattering lengths of the states $|1\rangle$ and $|2\rangle$ are known to be in the proportion $a_{11}:a_{12}:a_{22} = 1.03:1.0:0.97$ with the average of the three being $55(3)$ Å. They found that when the minima of the trapping potentials V_1 and V_2 are displaced from each other by a distance which is small compared to the size of the total condensate the resulting separation of the centres of mass of the condensates is much larger [1]. In this paper we provide for an analytical and numerical explanation for this result.

The basic physics of this amplification of the trap centre difference comes from the two possible final configurations of the mixture and that the system is close to the ‘critical point’ that separates the two final configurations; essentially the same idea in modern electronics where amplification comes from being close to the ‘critical point’ of the feedback loop. The two configurations are the symmetric one where one component is inside and the other component is outside and the asymmetric one [3–5] where the two components are on opposite sides. The former configuration is favoured when $\kappa = \sqrt{a_{11}/a_{22}}$ is different from one, with the less repulsive component in the middle where the density is higher. The asymmetric configuration possess a lower interface energy and is favoured when κ is close to one. We find that in the Thomas–Fermi approximation (TFA), when the trapping frequencies for the two components are the same, the amplification factor is proportional to $1/(\kappa - 1)$.

We also find that the relative magnitude of the critical angular velocity to generate vortices in the inner and the outer condensates changes as the trap centres are moved apart. This effect remains to be investigated experimentally. We now explain our results in detail.

In order to explore the boundary between the two condensates, we begin with the analysis of their behaviour in the framework of the TFA, which ignores the kinetic energy terms in the Gross–Pitaevskii equations for the condensate wavefunctions [8].

In dimensionless variables, the Gross–Pitaevskii equations for the condensates in the harmonic traps may be written in the form

$$-\nabla'^2 \psi'_1 + (x'^2 + y'^2 + \lambda^2(z' + z'_0)^2) \psi'_1 - \mu'_1 \psi'_1 + u_1 |\psi'_1|^2 \psi'_1 + \frac{8\pi a_{12} N_2}{a_\perp} |\psi'_2|^2 \psi'_1 = 0 \quad (1)$$

$$-\nabla'^2 \psi'_2 + (x'^2 + y'^2 + \lambda^2(z' - z'_0)^2) \psi'_2 - \mu'_2 \psi'_2 + u_2 |\psi'_2|^2 \psi'_2 + \frac{8\pi a_{12} N_1}{a_\perp} |\psi'_1|^2 \psi'_2 = 0. \quad (2)$$

Here $\psi_i(\mathbf{r}) = \sqrt{N_i/a_\perp^3} \psi'_i(\mathbf{r}')$, $\psi_i(\mathbf{r})$ is the wavefunction of the species i of a two-species condensate ($i = 1, 2$). $\lambda = \omega_z/\omega$. $\mathbf{r} = a_\perp \mathbf{r}'$, where $a_\perp = (\hbar/m\omega)^{1/2}$. ω is the trapping frequency. $\mu'_i = 2\mu_i/\hbar\omega$, where μ_i is the chemical potential of the species i . The chemical potentials μ_1 and μ_2 are determined by the relations $\int d^3 |\psi_i|^2 = N_i$. u_i is given by $u_i = 8\pi a_{ii} N_i/a_\perp$. The wavefunction $\psi'_i(\mathbf{r}')$ is normalized to 1. z'_0 denotes the shift of the minimum of the trapping potential in the vertical direction.

Equations (1) and (2) were obtained by minimization of the energy functional of the trapped bosons given by

$$E' = \frac{1}{2} \int d^3 r' \left[N_1 |\nabla' \psi'_1|^2 + N_1 (x'^2 + y'^2 + \lambda^2(z' + z'_0)^2) |\psi'_1|^2 \right. \\ \left. + N_2 |\nabla' \psi'_2|^2 + N_2 (x'^2 + y'^2 + \lambda^2(z' - z'_0)^2) |\psi'_2|^2 \right. \\ \left. + \frac{1}{2} N_1 u_1 |\psi'_1|^4 + \frac{1}{2} N_2 u_2 |\psi'_2|^4 + \frac{4\pi a_{12}}{a_\perp} N_1 N_2 |\psi'_1|^2 |\psi'_2|^2 \right]. \quad (3)$$

The energy of the system E is related to E' by $E = \hbar\omega E'$.

In the TFA, equations (1)–(3) can be further simplified by omitting the kinetic energy terms. In the framework of TFA the phase segregated condensates do not overlap, from equations (1) and (2) we obtain the simple algebraic equations

$$|\psi'_1(\mathbf{r}')|^2 = \frac{1}{u_1} (\mu'_1 - (r'^2 + \lambda^2(z' + z'_0)^2)) \Theta(\mu'_1 - (r'^2 + \lambda^2(z' + z'_0)^2)) \\ \times \Theta(r'^2 + \lambda^2(z' - z'_0)^2 - \mu'_2) \quad (4)$$

$$|\psi'_2(\mathbf{r}')|^2 = \frac{1}{u_2} (\mu'_2 - (r'^2 + \lambda^2(z' - z'_0)^2)) \Theta(\mu'_2 - (r'^2 + \lambda^2(z' - z'_0)^2)) \\ \times \Theta(r'^2 + \lambda^2(z' + z'_0)^2 - \mu'_1). \quad (5)$$

Here Θ denotes the unit step function and $\rho'^2 = x'^2 + y'^2$. If $z'_0 = 0$, from equations (4) and (5) one can see that the condensate density has the ellipsoidal form. This case has been considered in detail in [6, 7].

In the case of phase separation, the energy of the system can be written in the form [6, 7] $E = E_1 + E_2$, where

$$E_1 = \frac{1}{2} \hbar\omega N_1 \left[\mu'_1 - \frac{1}{2} u_1 \int d^3 r' |\psi'_1|^4 \right] \quad (6)$$

$$E_2 = \frac{1}{2} \hbar\omega N_2 \left[\mu'_2 - \frac{1}{2} u_2 \int d^3 r' |\psi'_2|^4 \right]. \quad (7)$$

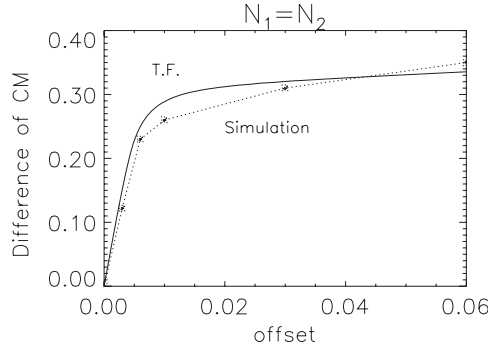


Figure 1. The distance between the centres of mass of the condensates (divided by the total length of the density distribution in the z direction) as a function of α for $N_1 = N_2$ from both the TF approximation and through numerical minimization of the energy functional.

To determine the position of the boundary between the condensates, we use the condition of thermodynamic equilibrium [9]: the pressures exerted by both condensates must be equal, $P_1 = P_2$. The pressure is given by [10] $P_i = G_{ii}|\psi_i|^4/2$, where $G_{ii} = 4\pi\hbar^2 a_{ii}/m_i$. Using these equations one can obtain the equation for the interface boundary

$$\rho'^2 + \left(\lambda z'' - \frac{\alpha(\kappa + 1)}{\kappa - 1} \right)^2 = R^2 \quad (8)$$

where $z' = \sqrt{\mu'_1} z''$, $\rho' = \sqrt{\mu'_1} \rho''$, $\alpha = \lambda z'_0$, and

$$R^2 = \frac{\mu'_1 - \kappa \mu'_2}{\mu'_1(1 - \kappa)} + \frac{4\alpha^2 \kappa}{(\kappa - 1)^2}. \quad (9)$$

As we emphasized in the introduction, the effective shift of the boundary in equation (8) is inversely proportional to $\kappa - 1$. Using normalization condition $\int |\psi'_i(\mathbf{r}')|^2 d^3 r' = 1$, one can determine the chemical potentials μ'_i as functions of N_1 , N_2 and α . The exact formulas for μ'_1 and μ'_2 obtained after tedious but straightforward calculations are rather cumbersome and will be given elsewhere. In this paper we discuss the results of the calculations. To be specific, we shall use the parameters corresponding to the experiments on ^{87}Rb atoms $a_{\perp} = 2.4 \times 10^{-4}$ cm, $N = N_1 + N_2 = 0.5 \times 10^6$ atoms, $\lambda = \sqrt{8}$.

In figure 1 we show the distance between the centres of mass of the condensates (divided by the total length of the density distribution in the z direction) as a function of α , calculated in the framework of TFA. In particular, for $\alpha = 0.03$ the separation of the centres of mass is 32% of the extent of the entire condensate. This value should be compared with the experimental quantity 20% [1]. The discrepancy between calculated and experimental values may partly be due to the effect of temperatures. To study if the accuracy of the TF approximation, we have minimized the full functional in equation (3). We use a Monte Carlo simulated annealing technique that has been described previously [4]. This scheme enables one to calculate configuration average of a physical quantity X defined by $\langle X \rangle = \sum_{\rho} \exp(-F/T) X(\rho) / \sum_{\rho} \exp(-F/T)$. We calculate $\langle X \rangle$ with decreasing T until the result stabilizes. In our calculation, we have used a mesh of $40 \times 40 \times 40$ sites, with 24 000 MC steps/site. The results for the centre of mass difference are shown in figure 1 (dotted curve). The agreement with the TF result is good.

From equations (8), (9) the evolution of the system upon increasing α may be described as follows: for $\alpha = 0$ condensate 1 forms the shell about the ellipsoidal condensate 2. The semiaxis of this ellipsoid is given by equation (8) for $\alpha = 0$. Upon increasing α the inner

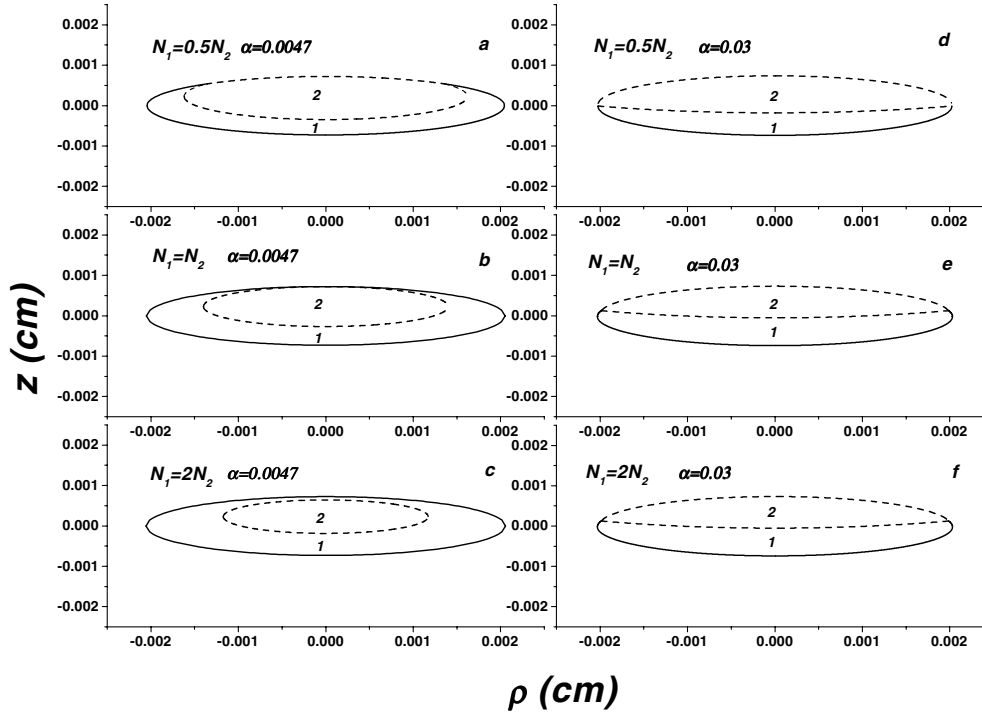


Figure 2. The cross sections of the condensate by the plane along the z -axis for different values of α and N_2/N_1 . Solid curves correspond to the border of the $|1\rangle$ atoms and dashed curves—the $|2\rangle$ atoms.

ellipsoid moves upwards, while external one moves down. It may be shown that they touch each other for the critical value of α : $\alpha_c = \frac{1}{2} \left(1 - \sqrt{\frac{\mu_2}{\mu_1}} \right)$. For $\alpha > \alpha_c$ phase boundary (8) intersect boundaries of condensates at the points with coordinates:

$$\lambda z_c'' = \frac{\alpha}{\kappa - 1} - \frac{(\kappa - 1)(R^2 - 1)}{4\alpha\kappa} \quad (10)$$

$$r_{1,2}'' = \pm \sqrt{1 - (\lambda z_c'' + \alpha)^2} \quad (11)$$

which can be obtained from equations (4)–(8).

Figure 2 illustrates the behaviour of the condensates for different values of α and N_2/N_1 . In figure 2 we show the cross-section of the condensate by the plane along the z -axis. $\alpha = 0.0047$ is equal to the critical value of α for $N_1 = N_2$. From figures 2(a)–(c) one can see that for $N_2/N_1 = 0.5$ $\alpha = 0.0047$ is less than the critical value, but for $N_2/N_1 = 2$ it is larger than the critical value. $\alpha = 0.03$ (approximately 3% of the extent of the density distribution in the vertical direction) corresponds to the experimental situation in [1]. One can see that when α increases, the phase boundary becomes more flat. It should be noted that rather small shifts of the trapping potential centres with respect to each other produce considerable changes of the form of the phase boundary.

The density distribution obtained from minimization of the full functional for $N_1 = N_2$ are illustrated in figure 3 where we show the contour plots of the two densities (solid and dashed curves) as a function of x and z for $y = 0$ for $\alpha = 6, 0.6\%$. The finite extent of the interface domain boundary is obvious.

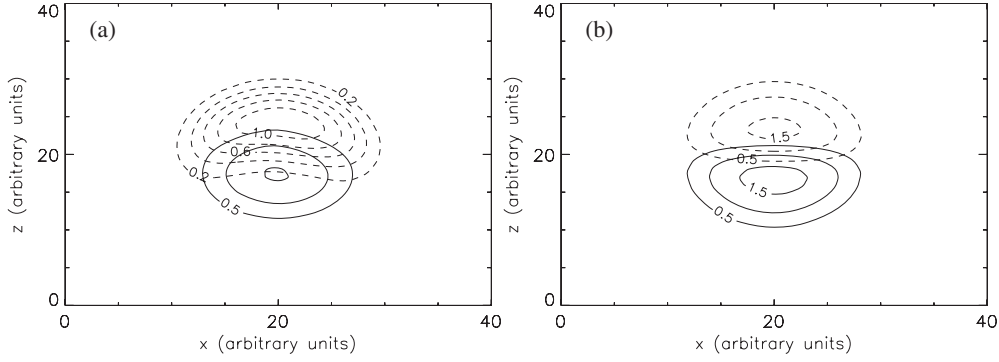


Figure 3. Counter plots of the density of the two components as a function of z and x for $y = 0$ for (a) $\alpha = 0.006$ and (b) $\alpha = 0.06$.

Another interesting question is how the vortex states change when the minima of the trapping potentials V_1 and V_2 are displaced with respect to each other. In a frame rotating with the angular velocity Ω along the z -axis the energy functional of the system is

$$E_{\text{rot}}(l_1, l_2) = E(\psi_{l_1}, \psi_{l_2}) + \int d^3r (\psi_{l_1}^* + \psi_{l_2}^*) i\hbar\Omega \partial_\phi (\psi_{l_1} + \psi_{l_2}) \quad (12)$$

where $\psi_{l_j}(\mathbf{r}) = |\psi_{l_j}(\mathbf{r})|e^{il_j\phi}$ is the wavefunction for the vortex excitation with angular momentum $\hbar l_j$. In the TFA, the vortex induced change in condensate density is negligible [11] (hydrodynamic approximation).

In the case of the phase segregated condensate, one finds from equations (12) and (6), (7) that the energy change due to presence of the vortices $\Delta E = E_{\text{rot}}(l_1, l_2) - E_{\text{rot}}(0, 0)$ has the form

$$\Delta E = \Delta E_{N_1} + \Delta E_{N_2} = \frac{1}{2}\hbar\omega_1 N_1 \int d^3r' \left(\frac{l_1^2}{\rho'^2} |\psi_1'|^2 - \frac{2\Omega l_1}{\omega_1} |\psi_1'|^2 \right) + \frac{1}{2}\hbar\omega_1 N_2 \int d^3r' \left(\frac{l_2^2}{\rho'^2} |\psi_2'|^2 - \frac{2\Omega l_2}{\omega_1} |\psi_2'|^2 \right). \quad (13)$$

In the hydrodynamic limit ψ_i' is given by equations (4) and (5).

In the case $\alpha = 0$ critical velocities as functions of ratio N_2/N_1 have been calculated in [6]. It was shown that for all values of N_2/N_1 , the critical velocity Ω_{N_2} for the formation of vortices in the inner condensate is larger than the critical velocity Ω_{N_1} of the outer vortex. So upon increasing Ω , a vortex will appear first in the external condensate. However, if for a given Ω one shifts the centres of the trapping potentials with respect to each other in the vertical direction, the inner condensate expands radially. One expects that the critical velocities of the condensates become closer and even can be equal for some values of α and N_2/N_1 . Figure 4 shows the behaviour of critical velocities as functions of α for different values of N_2/N_1 . Dashed curves correspond to the inner condensate, solid curves—to outer one. From figure 4(c) one can see that the critical velocities really can intersect. Physically this means that there is the possibility to exchange the vortex states between condensates by shifting the centres of the trapping potentials with respect to each other for fixed angular velocities.

In summary, we have shown that for simultaneously trapped condensates consisting of ^{87}Rb atoms in two different hyperfine states the small displacement of the minima of the trapping potentials with respect to each other produces profound effects on the phase separation and vortex states. The behaviour of the centres of mass of the condensates which follows from

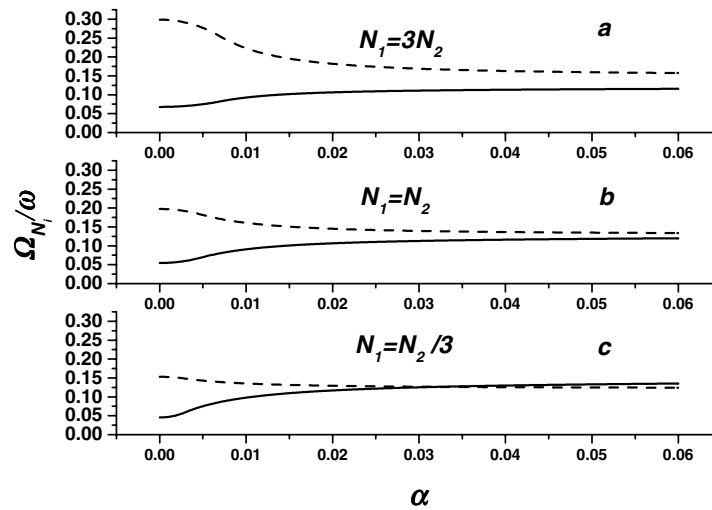


Figure 4. Critical velocities of outer condensate Ω_{N_1}/ω and the inner condensate Ω_{N_2}/ω as functions of α for different values of N_2/N_1 . Dashed curves correspond to Ω_{N_2}/ω and solid curves to Ω_{N_1}/ω .

our results is in agreement with the experiment by Hall *et al* [1]. The predicted possibility of the vortex states exchange between condensates due to the shift of the trapping potentials remains to be investigated experimentally.

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