Effects of Axial Vorticity in Elongated Mixtures of Bose-Einstein Condensates

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We consider a meniscus between rotating and nonrotating species in the Bose-Einstein condensate (BEC) with repulsive inter-atomic interactions, confined to a pipe-shaped trap. In this setting, we derive a system of coupled one-dimensional (1D) nonpolynomial Schrödinger equations (NPSEs) for two mean-field wave functions. Using these equations, we analyze the phase separation/mixing in the pipe with periodic axial boundary conditions, i.e. in a toroidal configuration. We find that the onset of the mixing, in the form of suction, i.e., filling the empty core in the vortical component by its nonrotating counterpart, crucially depends on the vorticity of the first component, and on the strengths of the inter-atomic interactions.

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Since the creation of vortices in Bose-Einstein condensates (BECs)\textsuperscript{[1, 2]}, this topic has been a subject of many experimental and theoretical works, as reviewed in Refs. \textsuperscript{[3]}. In particular, much attention has been drawn to vortices in mixtures of two BEC species; in fact, the first vortices were created in a two-component setting \textsuperscript{[1]}, and a theoretical analysis of that setting was developed too \textsuperscript{[4]}. In this connection, a situation of straightforward interest is the interaction of rotating and nonrotating immiscible BEC species. It is natural to expect that the nonrotating component may fill the hollow vortical core(s) in the rotating one. As shown experimentally, vortices and vortex lattices with empty and filled cores feature a great difference in their structure \textsuperscript{[2, 5]}. Very recently it has been also predicted the possibility to create vortex with arbitrary topological charge by phase engineering \textsuperscript{[6]}

Matter-wave vortices can be created not only in large-aspect ratio settings, but also in narrow cigar-shaped traps (“pipes”), which help to stabilize them \textsuperscript{[7]}. In the pipe geometry, it is interesting to consider the interaction of rotating and nonrotating BEC species, which is the subject of the present work. In particular, a natural issue in this case is the effect of “suction”, i.e., onset of effective mixing between two nominally immiscible species by pushing the nonrotating component into the empty core in the vorticity-carrying one. In other words, the suction implies indefinite stretching of the meniscus separating the immiscible species which originally fill two halves of the tube.

In the mean-field approximation, the starting point of the analysis is a system of coupled Gross-Pitaevskii equations (GPEs) for macroscopic wave functions, $\psi_1$ and $\psi_2$, of the two BEC species confined in the tight cylindrical trap. In the scaled form, the equations are

$$i \frac{\partial \psi_1}{\partial t} = \left[ -\frac{1}{2} \nabla^2 + \frac{1}{2} (x^2 + y^2) + \left( g_1 |\psi_1|^2 + g_{12} |\psi_2|^2 \right) \right] \psi_1,$$

$$i \frac{\partial \psi_2}{\partial t} = \left[ -\frac{1}{2} \nabla^2 + \frac{1}{2} (x^2 + y^2) + \left( g_2 |\psi_2|^2 + g_{12} |\psi_1|^2 \right) \right] \psi_2,$$

where $z$ is the axial coordinate, while $x$ and $y$ are the transverse ones. In these equations, lengths are measured in units of $a_{12}^{(1)} = \sqrt{\hbar/(m_1 \Omega_1)}$, the energy in units of $\hbar \Omega_1$, and time in units of $1/\Omega_1$, where $m_{1,2}$ and $\Omega_{1,2}$ are masses and transverse trapping frequencies of the two species, while the relative parameters in Eqs. (1) and (2) are $m = m_2/m_1$ and $\Omega = \Omega_2/\Omega_1$. The interaction strengths in the equations are expressed in terms of the s-wave inter-atomic scattering lengths, $g_{12} \equiv 2a_{12}/a_{12}^{(1)}$, $g_{12} \equiv 2a_{12}/a_{12}^{(1)}$, where $a_j$ is the scattering length in the $j$-th species, while $a_{12}$ is the scattering length for atoms belonging to the different species. In this work, we consider the most relevant situation with the repulsion between atoms belonging to the same and different species, i.e., we take $g_{1, g_2, g_{12}} > 0$.

We will solve equations (1) and (2), as well as effective 1D equations to be derived from them, with periodic boundary conditions in the axial direction ($z$), which assumed that the pipe is closed into a torus of large radius. Toroidal traps of the magnetic type are currently available to the experiment \textsuperscript{[8]}, and the BEC dynamics in the toroidal geometry was studied theoretically in several works \textsuperscript{[9]}. Actually, a variety of the toroidal configuration is a skyrmion pattern predicted in a two-component BEC, in which one component, which carries the vorticity, is effectively trapped in a doughnut region created by the other component, the entire configuration being stable \textsuperscript{[10]}

Equations (1) and (2) conserve the norms of the two wave functions, i.e., numbers of atoms in the species, $\int |\psi_{1,2}(r, t)|^2 \, dr = N_{1,2}$. The conserved energy (Hamil-
It is well known that, in the case of repulsion between atoms, the two species in the free space are miscible under the condition $g_{12}/(g_1 g_2) < 1$, and miscible in the opposite case \[11\]. The pressure induced by the transverse confinement changes the situation, pushing the system towards stronger miscibility (see, e.g., Ref. \[12\]).

We aim to study a different effect, \textit{viz.}, a shift of the miscibility threshold induced by vorticity imparted to one of the species. First, we derive a system of effective one-dimensional (1D) nonpolynomial Schrödinger equations (NPSEs) for the rotating and nonrotating species trapped in the pipe. The derivation extends the earlier developed analysis of the single-component \[13\] and two-component \[14\] settings, as well as the single-component case with the vorticity \[15\]. Then, the coupled NPSEs are used to predict, in an analytical form, the threshold for the transition to the immiscibility in the mixture including the rotating and nonrotating components. Finally, the prediction is compared to direct numerical solutions of the 3D equations, \[1\] and \[2\], which demonstrates a high accuracy of the analytical miscibility condition. Actual mixed and phase-separated configurations, and the onset of suction, are presented using numerical solutions of the 3D equations.

Coupled GPEs \[1\] and \[2\] can be derived from the action functional,

$$ S = \int dt \int d\mathbf{r} \left\{ -E + \frac{i}{2} \int \left( \psi_1 \frac{\partial}{\partial t} \psi_1 + \psi_2 \frac{\partial}{\partial t} \psi_2 \right) \right\}, $$

with $E$ taken as per Eq. \[3\]. To derive effective 1D equations in the axial direction ($z$), we generalize the 3D ansatz proposed for nonrotating configurations in Ref. \[14\], assuming that the vorticity, which is quantified by integer positive “spin” $S$, is imparted to the first species, while the second species has no vorticity:

$$ \psi_1(r,t) = \frac{(x^2 + y^2)^{S/2}}{\sqrt{\pi S!} \sigma_1(z,t)^{S+1}} \exp \left( i S \theta - \frac{x^2 + y^2}{2\sigma_1^2(z,t)} \right) f_1(z,t), $$

$$ \psi_2(r,t) = \frac{1}{\sqrt{\pi \sigma_2(z,t)}} \exp \left( -\frac{x^2 + y^2}{2\sigma_2^2(z,t)} \right) f_2(z,t), $$

denoting the model's effective action functional. Extremizing this functional with respect to $f_1(z,t)$ and $f_2(z,t)$ (the asterisk stands for the complex conjugation), we derive the coupled time-dependent NPSEs,

$$ \frac{\partial f_1}{\partial t} = \left[ \frac{\partial^2}{\partial z^2} + \frac{S + 1}{2} \frac{1}{\sigma_1^2} \right] f_1(z,t), $$

$$ \frac{\partial f_2}{\partial t} = \left[ \frac{1}{2m} \frac{\partial^2}{\partial z^2} + \frac{1}{2} \frac{1}{\sigma_2^2} + \Omega^2 \frac{\sigma_2^2}{\sigma_1^2 + \sigma_2^2} \right] f_2(z,t). $$

In addition, two relations are generated by varying the effective action functional with respect to $\sigma_1, \sigma_2$,

$$ \sigma_1 = 1 + \frac{(2S)!}{(S + 1)2^{2S}(S!)^2} \frac{g_1}{2\pi} \left| f_1(z,t)^2 + \frac{2g_2}{\pi(\sigma_1^2 + \sigma_2^2)^{S+2}} \right| f_2(z,t)^2, $$

$$ \Omega^2 \sigma_2^2 = \frac{1}{m} + \frac{g_2}{2\pi} \left| f_2(z,t)^2 + \frac{2g_1}{\pi(\sigma_1^2 + \sigma_2^2)^{S+2}} \right| f_1(z,t)^2 - 2S \frac{g_1}{\pi(\sigma_1^2 + \sigma_2^2)^{S+2}}. $$

In the absence of vorticity in the first species, $S = 0$, Eqs. \[7\], \[8\], \[9\], \[10\] reduce to those recently derived in Ref. \[14\] for the nonrotating two-component mixture.

In the case of $g_{12} = 0$ the two components decouple and we obtain the NPSE for the single-component BEC under transverse harmonic confinement, carrying axial vorticity $S \in \mathbb{Z}$. With $S = 0$, the equation reduces to the NPSE originally derived in Ref. \[13\]. The single-component model with $S \neq 0$ was recently studied in Ref. \[15\].

To analyze how the well-known phase-separation condition in the free space is modified in the pipe-shaped toroidal trap (\textit{i.e.,} as said above, we assume periodic boundary conditions in the direction of $z$), we consider the following initial expression for a weak perturbation of the axially uniform configuration (\textit{i.e.,} a fully mixed one), $f_{1,2}(z) = \sqrt{n_1,2} \left[ 1 \pm \alpha \cos (z/R) \right]$, where $n_1$ and $n_2$ are densities of the two components in the unperturbed state, $\alpha$ and $\beta$ the perturbation amplitudes, and $R$ the radius of the torus. Inserting these functions into expression \[3\], we find a correction to the effective energy at the second order in $\alpha$ and $\beta$,

$$ E_2 = \frac{n_1}{(4\pi R)^2} + \frac{(2S)!}{2^{2S}(S!)^2 8\pi \sigma_1^2} \alpha^2. $$
The critical curve of the phase separation is determined by equating the energy curvature to zero, which yields

\[ \frac{\sigma_2^{2S}}{(\sigma_1^2 + \sigma_2^2)^{2S+2}} g_{12} = \frac{(2S)!}{2^{2S+2}(S!)^2 \sigma_2^2} g_1 g_2 \]

\[ + \frac{\pi}{8m_1 n_2 R^2} \left[ \frac{(2S)! n_2 g_2}{2^{2S}(S!)^2 \sigma_1^2} + \frac{n_1 g_2}{\sigma_2} + \frac{\pi}{2m R^2} \right]. \quad (11) \]

From this condition it follows that, even for \( g_1 = g_2 = 0 \) (no intra-species repulsion, while the inter-species repulsion is in the action), the mixed state exists if the value of the coefficient \( g_{12} \) accounting for the repulsion between the species, is below a critical value, i.e. if:

\[ g_{12} < g_{12}^{(c)} = \frac{\pi}{4 \sqrt{m_1 n_2} R^2} \frac{(\sigma_1^2 + \sigma_2^2)^S}{\sigma_2^{2S}}. \quad (12) \]

This is clearly a finite-size effect, since expression \( (12) \) vanishes at \( R \to \infty \).

If the density is small enough, relations \( (9) \) and \( (10) \) may be approximated by \( \sigma_1 \approx 1 \) and \( \sigma_2 \approx 1/(m_1^{1/4} m^{-1/2}) \), and Eq. \( (11) \) yields a simple explicit result, in the limit of \( R \to \infty \), for the onset of the "suction" effect (uniform density of the two species along \( z \)):

\[ g_{12}^{(c)} = \frac{(2S)!}{2^{2S+2}(S!)^2} \frac{(m_1^{1/2} + 1)^{2S+2}}{m_1^{1/2} \Omega}. \quad (13) \]

In the absence of axial vorticity \( (S = 0) \), and for the two species with the same mass \( \langle m \rangle = 1 \) and common strength of the transverse confinement \( \Omega = 1 \), Eq. \( (13) \) coincides with its counterpart for the free \( (3D) \) space, \( g_{12}^{(c)} / (g_1 g_2) = 1 \).

We have tested condition \( (13) \) against direct numerical solutions of the full 3D equations, \( (1) \) and \( (2) \). Results of the comparison are displayed in Fig. 1 which shows that the analytical criterion \( (13) \) for phase separation is very accurate, at least up to \( g_1 N = 10 \).

We report also typical demixed (phase-separated) and mixed states, obtained as direct numerical solutions of Eqs. \( (1), (5), (9), (10) \) with periodic boundary conditions along \( z \), to model the torus of a large radius. If the radius is much larger than the transverse width \( \alpha_\perp \), effects of the curvature in the axial direction may be neglected \( (10) \). We solved the equations numerically by means of a finite-difference Crank-Nicholson predictor-corrector method with the cylindrical symmetry (details of the method were given in Ref. \( (20) \)). To generate the ground-state wave functions \( \psi_{1,2}(r, z) \), with \( j = 1, 2 \), the imaginary-time integration was used.

In Fig. 2 we plot typical examples of the axial and radial densities,

\[ \rho_j(z) = N_j^{-1} \int_0^\infty 2\pi r dr |\psi_{j,2}(r, z)|^2, \quad (14) \]
FIG. 3: (Color online). The axial densities $\rho_j(z)$ of the two components of the binary BEC in the quasi-1D toroidal trap for two values of the axial length, $L = 40$ and $L = 400$. The continuous and dashed curves represent the first and second components. The parameters are $m = \Omega = 1$, $N_1 = N_2 = N$, $g_1 N = g_2 N = 1$, $g_{12} N = 30$, $S = 0$.

$$\rho_j(r) = N_j^{-1} \int_{-\infty}^{+\infty} dz |\psi_{1,2}(r,z)|^2, \quad j = 1, 2.$$  \hspace{1cm} (15)

Figure 2 displays the demixing (phase separation) for $S = 0$ and $S = 1$, while no separation is observed in the axial direction for $S = 2$. In fact, this means that the empty core induced by the vorticity with $S = 2$ is wide enough to produce the “suction” effect, while $S = 1$ is not sufficient for that.

To further illustrate the situation, in Fig. 3 we plot the axial density profiles of the two components of the binary BEC in the regime of the phase separation for two different values of the axial length, $L = 2\pi R = 40$, and $L = 400$, i.e., “short” and “long” tori, respectively. The figure shows that the density profiles get flatter and interfaces steeper with the increase of $L$. In fact, for very large $L$ the contribution (generated by the gradient terms) to the total energy \([3]\) from to the interfaces become negligible in comparison with the bulk terms (the Thomas-Fermi approximation), the corresponding axial profiles looking as step functions. In this limit, the onset of phase separation is accurately described by Eq. \([13]\).

In conclusion, we have considered dynamical states in the binary BEC formed by two species with repulsion between atoms, in the case when one species is prepared in a vortical state, with vorticity $S = 1$ or 2, while the other has zero vorticity. It is assumed that the condensate was loaded in a quasi-1D toroidal trap, i.e., the corresponding equations were solved with periodic boundary conditions in the axial direction. In this setting, we have derived coupled 1D nonpolynomial Schrödinger equations (NPSEs) for the mean-field wave functions of the two components. Using these equations, we have found the phase-separation threshold, as a condition for the onset of the modulational instability of axially uniform states. The predictions produced by the NPSEs were compared to results of direct simulations of the underlying 3D equations, demonstrating a very good agreement. Further, stable 3D states with the species mixed and separated in the axial direction were found, the transition to the effective mixing being accounted for by the suction, i.e., filling the empty core in the vortical component by the nonrotating one. The onset of the suction depends on the size of the vorticity in the first component, and on the relative strength of the inter-species repulsion in comparison with the intrinsic repulsion in each component.
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