Matter-wave vortices in cigar-shaped and toroidal waveguides

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We study vortical states in a Bose-Einstein condensate (BEC) filling a cigar-shaped trap. An effective one-dimensional (1D) nonpolynomial Schrödinger equation (NPSE) is derived in this setting, for the models with both repulsive and attractive inter-atomic interactions. Analytical formulas for the density profiles are obtained from the NPSE in the case of self-repulsion within the Thomas-Fermi approximation, and in the case of the self-attraction as exact solutions (bright solitons). A crucially important ingredient of the analysis is the comparison of these predictions with direct numerical solutions for the vortex states in the underlying 3D Gross-Pitaevskii equation (GPE). The comparison demonstrates that the NPSE provides for a very accurate approximation, in all the cases, including the prediction of the stability of the bright solitons and collapse threshold for them. In addition to the straight cigar-shaped trap, we also consider a torus-shaped configuration. In that case, we find a threshold for the transition from the axially uniform state, with the transverse intrinsic vorticity, to a symmetry-breaking pattern, due to the instability in the self-attractive BEC filling the circular trap.

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I. INTRODUCTION

An important setting for experimental and theoretical studies of dynamical phenomena in Bose-Einstein condensates (BECs) is provided by nearly one-dimensional (1D) “cigar-shaped” traps, which assumes tight confinement in the transverse plane, allowing to unravel the dynamics along the longitudinal axis. The use of this geometry helped to achieve famous experimental results, such as the creation of single \cite{1} and multiple \cite{2} bright solitons in the condensate of several thousand \textsuperscript{7}Li atoms. In those experiments, the strength of the interaction between atoms was controlled and made weakly attractive by means of the Feshbach-resonance technique. In the condensate of \textsuperscript{85}Rb atoms trapped in a similar geometry, nearly 3D solitons were found in a post-collapse state \cite{3}.

It is natural to derive effectively one-dimensional (1D) equation(s) for the description of this experimentally relevant setting, starting from the full 3D Gross-Pitaevskii equation (GPE). The reduction of the 3D equation to a 1D form was performed, under various assumptions, by means of sundry methods \cite{4}-\cite{8}. In the simplest approximation, the difference of the eventual equation from a formal 1D variant of the GPE (with the underlying cubic nonlinearity) is represented by an additional quintic term, whose sign is always self-attractive, irrespective of the sign of the cubic nonlinearity \cite{6}. A more consistent approach to the derivation of the 1D equation postulates the factorization of the 3D mean-field wave function into the product of the ground state of the 2D harmonic oscillator in the transverse plane, and slowly varying axial (1D) wave function. Using the variational representation of the underlying 3D GPE, this approach ends up with the nonpolynomial Schrödinger equation (NPSE) for the axial wave function \cite{3,4,10,11}. The NPSE has been extended to investigate the Tonks-Girardeau regime \cite{12}, the two-component BEC \cite{13}, and also transverse spatial modulations \cite{14}.

Another physically interesting modification of the above setting is that when the BEC trapped in the cigar-shaped geometry is lent vorticity (assuming that the corresponding vector of the angular momentum is directed parallel to axis of the cigar-shaped trap), as proposed in Ref. \cite{15}. In the experiment, the vorticity may be imparted on the condensate by a helical laser beam shining along the axis of the trap. A natural problem for the theoretical analysis, which is considered in the present work, is the derivation of a modification of the effective one-dimensional NPSE that takes into regard the intrinsic vorticity. As we demonstrate in Section II, such a modified 1D equation is not drastically different from its counterpart derived before \cite{3,4} for the zero-vorticity states. However, a really nontrivial issue is to compare basic dynamical states predicted by this effective equation with direct numerical solutions of the underlying GPE in three dimensions. In this work, we perform the comparison separately for the self-repulsive and self-attractive BEC (in Sections III and IV, respectively). In the former case, the relevant states are of the Thomas-Fermi (TF) type, while in the latter model (self-attraction) these are bright solitons. We demonstrate that the modified NPSE provides for very good approximation for all these states, including the prediction of their stability (and, in particular, of the collapse threshold for solitons in the self-attraction model). In addition, in Section V we consider a different geometry, when the long quasi-1D trap is bent...
and closed into a ring (torus), maintaining the intrinsic vorticity in the transverse plane. In that case, we find that the modified NPSE accurately predicts the shape and stability of a possible soliton, as well as the deformation transition to the state of the BEC uniformly filling the toroidal trap.

II. THE NONPOLYNOMIAL SCHRÖDINGER EQUATION (NPSE) FOR MATTER-WAVE VORTICES

The description of a dilute BEC, confined in the axial direction by a generic potential $V(z)$, and in the transverse plane by the harmonic potential with frequency $\omega_{\perp}$, is based on the fundamental GPE in three dimensions

$$i\frac{\partial \psi}{\partial t} = \left[ -\frac{1}{2} \nabla^2 + \frac{1}{2}(a^2 + g^2) + V(z) + 2\pi g|\psi|^2 \right] \psi, \tag{1}$$

where $\psi(r, t)$ is the macroscopic wave function of the condensate normalized to unity, and $g \equiv 2Na/a_{\perp}$, with $N$ the number of atoms, $a_{\perp} = \sqrt{\hbar/(m\omega_{\perp})}$ the length of the transverse harmonic confinement, and $a_{\perp}$ the scattering length of atomic collisions. In Eq. (1), the length and time units are $a_{\perp}$ and $\hbar\omega_{\perp}^{-1}$, and the energy unit is $\hbar\omega_{\perp}$.

This equation can be derived from the Lagrangian density:

$$\mathcal{L} = \frac{i}{2} \left( \psi^* \frac{\partial \psi}{\partial t} - \psi \frac{\partial \psi^*}{\partial t} \right) - \frac{1}{2} |\nabla \psi|^2 - \frac{1}{2} (a^2 + g^2)|\psi|^2 - V(z)|\psi|^2 - \pi g|\psi|^4. \tag{2}$$

In this work, we study the existence and properties of matter-wave states with vorticity in the transverse plane, which correspond to solutions of the form

$$\psi(r, t) = \Phi(r, z, t) e^{iS\theta}, \tag{3}$$

where $S$ is the integer vorticity quantum number, $r$ and $\theta$ being the polar coordinates in the $(x, y)$ plane. On the substitution of expression (3), Eq. (1) takes the form:

$$i\frac{\partial \Phi}{\partial t} = \left[ -\frac{1}{2} \left( \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{\partial^2}{\partial z^2} \right) - \frac{S^2}{2r^2} + \frac{1}{2} r^2 + V(z) + 2\pi g|\Phi|^2 \right] \Phi. \tag{4}$$

We solved Eq. (4) numerically by using the finite-difference Crank-Nicholson predictor-corrector method with the cylindrical symmetry described in Ref. [10]. The Crank-Nicholson algorithm with imaginary time is used to find the stationary wave function of the GPE with a fixed vorticity $S$. The algorithm provides for fast convergence to a finite-size wave function with finite energy.

In the case of instability due to collapse ($g < 0$) the algorithm quickly approaches a delta peak with (negative) diverging energy. Note that, in the free space, vortices are usually destroyed by the instability against azimuthal perturbations [17], which split them into a set of separating fragments [18], but in our setting this instability is suppressed by the tight transverse confinement.

To gain some analytical insight and to reduce the problem to 1-D, we apply a variational approach. In the case of a cigar-shaped geometry, it is natural to extend the variational representation [5, 9] of the 3D GPE which led to the NPSE for the axial wave function in the case of no vorticity to the present situation. Thus we adopt the following ansatz for the vortex state described by Eq. (4):

$$\Phi(r, z, t) = \frac{r^S}{\sqrt{\pi S!}} \sigma(z, t)^{S+1} \exp \left( -\frac{r^2}{2\sigma^2(z, t)} \right) f(z, t), \tag{5}$$

where $\sigma(z, t)$ and $f(z, t)$ which account for the transverse width and the amplitude of the vortex are to be determined variationally. By inserting this ansatz into the Lagrangian density (2) and performing the integration over $x$ and $y$, we derive the effective Lagrangian density,

$$\tilde{\mathcal{L}} = \frac{i}{2} f \frac{\partial f}{\partial z} - \frac{1}{2} \left( \frac{\partial f}{\partial z} \right)^2 - \frac{1}{2}(S+1) \left( \frac{1}{\sigma^2} + \sigma^2 \right) |f|^2 - \frac{1}{2}(S+1)gs |f|^4,$$

where the effective nonlinearity strength for the vortex state is

$$gs = g \frac{(2S)!}{2^{2S}(S+1)!S!^2}.$$

Note that the effective Lagrangian density (6) does not contain time derivatives of $\sigma(z, t)$. Expression (6) gives rise to the corresponding Euler-Lagrange equations,

$$i\frac{\partial f}{\partial z} = \left[ -\frac{1}{2} \frac{\partial^2}{\partial z^2} + V(z) + \frac{1}{2}(S+1) \left( \frac{1}{\sigma^2} + \sigma^2 \right) \right] f,$$

$$\sigma^4 = 1 + gs|f|^2 + \sigma^2 + \frac{\sigma^3}{|f|^2} \frac{\partial}{\partial z} \left( \frac{\sigma'}{\sigma^2} |f|^2 \right),$$

where $\sigma' \equiv \partial \sigma/\partial z$. Neglecting this derivative, Eqs. (7) and (8) can be combined into:

$$i\frac{\partial f}{\partial z} = \left[ -\frac{1}{2} \frac{\partial^2}{\partial z^2} + V(z) + (S+1) \frac{1 + (3/2)gs|f|^2}{\sqrt{1 + gs|f|^2}} \right] f,$$

which is a new version of the nonpolynomial Schrödinger equation (NPSE) for the vortical state tightly confined in the transverse plane. In the case of $S = 0$, Eq. (9) reduces to the ordinary NPSE, that has found various applications [3, 14].

The eigenfunctions of the equation

$$\left[ -\frac{1}{2} \frac{\partial^2}{\partial z^2} + V(z) + (S+1) \frac{1 + (3/2)gs|\phi|^2}{\sqrt{1 + gs|\phi|^2}} \right] \phi = \mu \phi \tag{10}$$


provide the stationary solutions of Eq. (9) of the form \( f(z,t) = \phi(z) e^{-i\mu t} \). Obviously, Eqs. (9) and (10) can be transformed into their counterparts for \( S = 0 \) by substitutions \( g \to g_S, \mu \to \mu/(S+1), t \to (S+1)t, z \to \sqrt{S+1}z, \) and \( V \to V/(S+1) \). Therefore, the results obtained in earlier works in the framework of the three-dimensional GPE for vortical states.

Equations (10). A really nontrivial issue is to compare these results with those produced by numerical integration of the full three-dimensional GPE for vortical states.

III. REPULSIVE NONLINEARITY

In the case of a repulsive inter-atomic interactions (i.e. \( g > 0 \)) one may readily generalized the TF approximation developed in Ref. [10], for \( S = 0 \) to the case with vorticity \( S \). Thus, neglecting the kinetic-energy term, i.e., the second derivative, in Eqs. (10) one gets the analytical expression for the stationary axial probability density \( \rho(z) = |\phi(z)|^2 \) in the form:

\[
\rho(z) = \frac{2}{g\phi_S} \left[ \mu^2_S(z) - 3 + \mu_S(z) \sqrt{\mu^2_S(z) + 3} \right],
\]

where the effective local chemical potential is

\[
\mu_S(z) = -\frac{\mu - V(z)}{S + 1}.
\]

Notice that generally expression (11) does not represent a soliton. Equations (11) and (12) are a straightforward generalization of the TF approximation developed in Ref. [10] for the repulsive BEC with \( S = 0 \).

To test the accuracy provided by the NPSE in this case, in Fig. 1 we plot the axial and radial probability densities of the repulsive BEC with vorticity \( S \), defined, respectively, as

\[
\rho(z) = \int_{-\infty}^{+\infty} |\psi(r,z)|^2 2\pi r dr,
\]

\[
\rho(r) = \int_{-\infty}^{+\infty} |\psi(r,z)|^2 dz,
\]

and obtained from the numerical solution of the stationary version of Eq. (11). They are compared with predictions of the stationary NPSE (10), as well as with analytical result (11) produced by the TF approximation. We choose \( g = 20 \), and take \( V(z) = z^2/2 \). This choice of the axial potential implies that the full potential is isotropic. Thus, we are testing the NPSE in a geometry far from the cigar-shaped one where it is expected to be very accurate, as it was verified in the case \( S = 0 \).

Figure 1 shows that, for all \( S \), the agreement between the 3D GPE and the NPSE (solid and dashed lines, respectively) is extremely good in the axial direction. There are some differences in the radial probability density, \( \rho(r) \). Remarkably, the TF version of the NPSE, i.e., Eq. (11) (which corresponds to the dotted-dashed line in the figure) also provides for very good accuracy of the axial probability-density distribution in the core of the confined space.

The comparison between the full GPE and the effective NPSE is further presented in Table 1, which displays values of the ground-state energy of the repulsive BEC with vorticity \( S \), as obtained from the three-dimensional GPE (\( E_{GPE} \)), and from the NPSE (\( E_{NPSE} \)). The former energy is calculated as

\[
E = \int \frac{1}{2} (V(z) + V^2 + \frac{1}{2} \Phi^2 + 3 \pi g |\Phi|^4) d^3 r,
\]

where \( \Phi(r) \) is the ground-state stationary solution of the GPE in the 3D setting. The energy \( E_{NPSE} \) is also obtained from Eq. (11), but with \( \Phi(r) \) corresponding to the ground-state stationary solution of the NPSE. The third column in the table shows that the relative error \( \Delta E_{NPSE}/E_{GPE} \) is quite small, and moreover that decreases with the increase of \( S \).

| \( S \) | \( E_{GPE} \) | \( \Delta E_{NPSE}/E_{GPE} \) | \( \Delta E_{TF}/E_{GPE} \) |
|-----|----------|----------------|----------------|
| 0   | 3.0729   | 0.0194         | 0.1855         |
| 1   | 3.6704   | 0.0071         | 0.2558         |
| 2   | 4.4878   | 0.0070         | 0.2295         |

Table 1. Repulsive Bose-Einstein condensate with nonlinearity strength \( g = 20 \) and vorticity \( S \), in axial trapping potential \( V(z) = z^2/2 \). \( E_{GPE} \) represents the ground-state energy as found from the full 3D GPE. \( \Delta E_{NPSE}/E_{GPE} \) and \( \Delta E_{TF}/E_{GPE} \) are the relative differences of \( E_{GPE} \) with respect to the ground state energy of NPSE and TFGPE wave functions.

In addition, we have also calculated the size of the term \( (S+1)\sigma^2/\sigma^2 \) in the effective Lagrangian (10), that
was neglected in the derivation of the NPSE. The result is that the neglected term is very small indeed, being always less than 0.5% of the energy produced by the NPSE.

For the sake of completeness, we have also calculated the axial probability density obtained by the application of the TF approximation to the full 3D GPE (TFGPE) and subsequent integration over \( x \) and \( y \). It is given by

\[
\rho(z) = \frac{1}{2g} \mu(z) \sqrt{\mu(z)^2 - S^2} \frac{S^2}{2g} \ln \left[ \frac{\mu(z) + \sqrt{\mu(z)^2 - S^2}}{\mu(z) - \sqrt{\mu(z)^2 - S^2}} \right],
\]

where \( \mu(z) = \mu - V(z) \). The left panels of Fig. 1 show that the results provided by this TFGPE approximation are slightly better than those obtained by the same approximation applied to the NPSE, but the full solution of NPSE is better than the TFGPE approximation, as shown in the last column of Table 1 and also in the left panels of Fig. 1, where the NPSE curves practically coincide with their counterparts produced by the numerical solutions of the GPE in 3D.

**IV. ATTRACTIVE NONLINEARITY**

Proceeding to the attractive inter-atomic interactions, i.e., negative \( g \) (and \( g_S \)), it is relevant to recall that, for \( V(z) = 0 \) and \( S = 0 \), a family of bright-soliton solutions to Eq. (9) was constructed in Refs. [5, 9]. In the case of \( S \neq 0 \), one is dealing with bright vortex solitons. In a numerical form, they were studied in Ref. [10]. A Gaussian-based variational approach was developed in Ref. [13], and, in a brief form [which resulted in an effective potential for the vortex soliton in the case of inhomogeneous transverse confinement, \( \omega_\perp = \omega_\perp(z) \)] also in Ref. [8]. The stability of the vortex solitons with both large and small aspect ratios (i.e., strongly elongated ones, as we consider here, or pancake-shaped solitons, tightly confined in the axial direction) was studied by means of accurate numerical methods, based on the linearization of the GPE with respect to small perturbations, in Refs. [17].

Here we use the NPSE in the form of Eq. (10) and compare its results with those from the full 3D GPE. To simplify the notation, we set

\[
\gamma_S = -|g_S| = -|g| \frac{(2S)!}{2^{2S} (S!)^2 (S + 1)},
\]

\[
\mu_S = \frac{\mu}{S + 1}.
\]

By imposing vanishing boundary conditions at infinity, \( \phi(z) \rightarrow 0 \) as \( z \rightarrow \pm \infty \), we find soliton solutions in an implicit analytical form,

\[
z \sqrt{2(1 + S)} = \frac{1}{\sqrt{1 - \mu_S}} \text{Arctanh} \left( \sqrt{1 - \gamma_S \phi^2} \frac{\gamma_S}{1 - \mu_S} \right).
\]

The soliton family is then characterized by the dependence of \( \gamma_S \) on \( \mu_S \). Eq. (15), implies that solitons do not exist if the nonlinearity strength exceeds the critical value, \( \gamma_S^{(c)} = 4/3 \), corresponding to \( \mu_S = 1/2 \). For stronger nonlinearities the NPSE [2] predicts a longitudinal collapse, that is a quantum tunneling to a high-density state [20] where atoms quickly evaporate due to three-body recombination [3]. In terms of the physical parameters, \( a < 0 \), \( a_\perp \), and \( N \) (number of atoms), we conclude that the collapse of the bright vortex soliton takes place in region

\[
\frac{N|a|}{a_\perp} > \frac{2 \ 2^{2S} (S!)^2 (S + 1)}{3 (2S)!}.
\]

As a final remark, we note that the inversion of Eq. (15) provides two branches of solutions for \( \mu_S(\gamma_S) \). In numerical simulations of Eq. (9), only the one satisfying the condition \( d\mu_S/d\gamma_S < 0 \) turns out to be stable, in precise agreement with the prediction of the Vakhitov-Kolokolov stability criterion [21].

In Fig. 2 we plot the axial probability density \( \rho(z) \) of the soliton with vorticity \( S \), with no axial external potential (\( V(z) = 0 \)), and for \( g = -1 \). The figure shows that the radial probability density \( \rho(r) \) produced by the NPSE is virtually indistinguishable from that generated by the 3D GPE. This can be understood since the system with \( g = -1 \) becomes effectively quasi-one-dimensional. The figure also shows that, for all \( S \), the agreement between the 3D GPE and the NPSE (solid and dashed lines) is excellent also in the axial direction. Thus, we conclude that the NPSE predicts the bright vortex solitons with a very high accuracy.

**V. VORTEX BRIGHT SOLITONS IN A RING**

Repulsive BECs in a ring-shaped (toroidal) trap are now available to the experiment [22]. Self-attractive BEC in a ring has not been experimentally created yet, but it may also be a promising setting, interesting from a physical point of view, since a quantum phase transition from a uniform state to a bright soliton has been predicted in Refs. [23]. This prediction is based on the mean-field and beyond-mean-field numerical analysis for the 1D Bose gas
with contact interactions and periodic boundary conditions. Recently, self-attractive BECs in a 3D ring-shaped trap were considered, taking into account the transverse structure of the trapped condensate. In this way, new features in the model’s phase diagram have been predicted, both at zero [24] and finite [25] temperatures.

The analysis presented in Refs. [24, 25] can be extended to the bright solitons with intrinsic vorticity by using the above-mentioned scaling transformation, to

\[ \phi(z + L) = \phi(z), \quad -L/2 < z < L/2, \]

where \( L = 2\pi R \) is the length of the ring with radius \( R \) (here, we do not assume any global vorticity imposed along the closed ring).

Equation (10) subject to the periodic b.c. always admits the axially uniform solution, \( \phi = 1/\sqrt{L} \). Further, in Ref. [24], it was shown that this uniform state, with \( S = 0 \), is energetically and dynamically stable in the attractive BEC only for a finite range of parameters. In the case of \( S \neq 0 \), the stability condition is modified, by the above-mentioned scaling transformation, to

\[ \frac{\pi^2}{\gamma S L \sqrt{S + 1}} \left( 1 - \frac{\gamma S}{L \sqrt{S + 1}} \right)^{3/2} \geq \left( 1 - \frac{3\gamma S}{4L \sqrt{S + 1}} \right), \]

which for large \( L \) reduces to

\[ \frac{\pi^2}{\gamma S L \sqrt{S + 1}} \geq 1. \] (17)

In terms of physical parameters, condition (17) takes the following form, cf. condition (16) for the onset of the collapse in the rectilinear trap:

\[ \frac{N|a|}{a_{\perp}} \leq \frac{\pi^2 a_{\perp} 2^{2S(S)} \sqrt{S + 1}}{2L (2S)!} \] (18)

FIG. 2: (color online). Axial \( \rho(z) \) and radial \( \rho(r) \) probability densities in the soliton state with vorticity \( S \), in the case of the self-attraction with strength \( g = -1 \) and \( V(z) = 0 \) (no axial potential). Solid lines: obtained from the full 3D GPE. Dashed lines: produced by the NPSE.

FIG. 3: Axial probability density \( \rho(z) \) in the state with transverse vorticity \( S \), in the ring-shaped waveguide, i.e., with the periodic boundary conditions in \( z \). Self-attraction strength is \( g = -1 \), and the length of the ring is 40. The results are obtained from the NPSE.

Note that in this inequality both the scattering length \( a \) and \( L \) are expressed in dimensional units.

In Fig. 3 we plot several profiles of the axial probability density \( \rho(z) \), as obtained from the NPSE, Eq. (9), with vorticity \( S \) and \( g = -1 \) (with no external axial potential: \( V(z) = 0 \)). Periodic boundary conditions are imposed, with period (length of the ring) \( L = 40 \). We have checked that, as well as in Fig. 2, the agreement between results produced by the 3D GPE and NPSE is very good for all \( S \) (we display only the profiles generated by the NPSE since they are indistinguishable in the figure from their counterparts obtained from the 3D equation). Note that, contrary to the case shown in Fig. 2, in the present case the axial probability density is uniform for \( S = 2 \), due to the delocalization transition, the threshold for which is very accurately predicted by Eq. (18).

VI. CONCLUSIONS

In this work, we have presented a systematic analysis of self-repulsive and self-attractive matter-wave patterns with the intrinsic vorticity which fill a straight or toroidal cigar-shaped trap. The 1D NPSE was derived from the underlying 3D GPE, as a modification of the previously derived 1D equation for the states without vorticity. In the cases of the self-repulsion and self-attraction, the modified NPSE predicts, respectively, the axial density profiles for the TF states and bright solitons, both in
an analytical form. The comparison of these predictions with direct numerical solutions of the underlying 3D GPE for the vortex states demonstrates a very high accuracy of the description provided by the NPSE, which includes the prediction of the stability of the bright solitons, as well as the threshold for the onset of collapse. For the toroidal configuration of the trap, a threshold for the transition from the axially uniform vortex state to a quasi-soliton symmetry-breaking pattern was found too.

This work may be naturally extended in several directions. In particular, a challenging problem is collision of solitons with opposite signs of the intrinsic vorticity, $+S$ and $-S$. This setting cannot be described by the NPSE (which assumes a single value of $S$ throughout the elongated trap), hence it should be studied in the framework of the full 3D GPE. Another interesting generalization may be formation of gap solitons with intrinsic vorticity, in the case when the nonlinearity is self-repulsive, and the cigar-shaped trap is combined with a periodic axial potential, like in the well-known experimental setting used for the creation of ordinary gap solitons [26].

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