Stability of vortices in inhomogeneous Bose condensates subject to rotation: A three-dimensional analysis

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We study numerically the stability of axially symmetric vortex lines in trapped dilute gases subject to rotation. For this purpose, we solve numerically both the Gross-Pitaevskii and the Bogoliubov equations for a three-dimensional condensate in spherically and cylindrically symmetric traps, from small to very large nonlinearities. In the stationary case we find that the vortex states with $m=1$ and $m=2$ are energetically unstable. In the rotating trap it is found that this energetic instability may only be suppressed for the $m=1$ vortex line, and that the multicharged vortices are never a local minimum of the energy functional. This result implies that the absolute minimum of the energy is not an eigenstate of the L_z operator, when the angular speed is above a certain value. [S1050-2947(99)03412-5]

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I. INTRODUCTION

Since the first experimental realization of Bose-Einstein condensation (BEC) in weakly interacting gases [1], there has been a large theoretical and experimental effort to study its properties in the framework of quantum field theories and in the so-called mean-field limit [Gross-Pitaevskii (GP) equations]. These equations are formally nonlinear Schrödinger equations (NLS) [2] and appear in many fields of physics, e.g., in bulk superfluids and nonlinear optics to cite only a few examples.

All of these physical systems have long been known to exhibit solutions with topological defects [3,4], of which the simplest ones are known as vortices (in two spatial dimensions) or vortex lines (in three spatial dimensions). Vortices are localized phase singularities with integer topological charge. Specifically, vortices appearing in the context of GP can be seen, in the framework of the hydrodynamic interpretation, to be analogous to the fluid dynamical vortices which appear in fluid dynamics [5]. In the framework of BEC studies, the question has been raised of whether these nonuniform clouds of condensed gases may support the existence of vortices in a stable form, and the purpose of this work is to help answer this question.

There is a huge amount of literature on vortices and vortex properties in the framework of NLS equations, including their particular cubic version (the GP equation), their nonconservative extensions [the Ginzburg-Landau (GL) system], and vector GL models. In particular, the stability of m-charged GP vortices in two dimensions was studied in [6]. In three dimensions, the GL case was recently considered [7] and geometric instabilities have been found to strongly deform the vortex lines. The results for the GL cannot be directly extrapolated to the GP equation since dissipation and diffusion are essential ingredients of the models studied in Ref. [7]. This fact makes the conservative case (GP) interesting by itself. Other analyses of vortices and of vortex stability in the framework of nonlinear optics are included in Ref. [8].

The current setups used to generate Bose-Einstein condensates utilize a magnetic trap to confine a highly cooled atomic cloud. This trap is mathematically modeled by a parabolic potential and distinguishes BEC from common NLS systems, in which the vortices are free and move in a homogeneous background. The dynamics of a vortex in a spatially inhomogeneous two-dimensional GP problem was studied in Ref. [9] using the method of matched asymptotic expansions, but the authors did not consider the stability of the two-dimensional (2D) vortex itself. In principle, the vortex motion equations of Ref. [9] can be used to study the motion of a single 2D point vortex in spatially inhomogeneous GP problems. However, the dynamics of the many-vortex case is more complicated and by no means trivial. For simple approaches to the problem which do not include the effect of vortex cores on the background field, see Ref. [10]. More elaborate analyses were done in Ref. [11]. An interesting discussion on the validity of the fluid approximation to the GP equation can be found in Ref. [12]. The dynamics of 3D vortices is yet more complicated, allowing the so-called reconnection. To our knowledge there are no analytical results but only qualitative numerical observations available [13]. Another theoretical framework in which nonhomogeneous dynamics of vortices has been investigated is the possibility of pinning vortices in type-II superconductors [14], but here the dynamics has been considered only through analytical approximation techniques with no comparison with numerics. In all the previously discussed cases, the stability of the vortex state is taken for granted.

The problem of vortex stability in the framework of Bose-Einstein condensed gases has been considered in various papers that address linear and global stability, either from a purely analytic point of view, such as in [15–18], or by mixing analytic and numerical techniques [20–23]. In Ref. [20], the authors solve the GP equation and find the energies of the condensate in vortex states, for a number of particles up to $N=10^4$. In Ref. [21], the authors solve the Bogoliubov equations for a unit charge vortex in a stationary trap with axial symmetry for populations of up to $N<10^4$ atoms. In Ref. [22], the authors perform stability calculations for a condensate with periodic boundary conditions on the Z axis, and study the influence of rotation in the energy and stability of the $m=1$ vortex. In Ref. [24], the authors address the problem of minimizing the energy functional with a reduced basis of trial states that is only valid in the limit of small U.

In this paper we unify and substantially extend what has been done in previous works regarding these two questions: global energetic stability and local stability of vortex states. First, in Sec. II we write the simplest equations that model a BEC in a possibly rotating trap and offer a variational point of view for the search of stationary states. In Sec. III we put forward the thesis that the ground state must have a well defined value of the third component of the angular momentum, $m=\langle L_z\rangle$, i.e., that it must be symmetric with respect to rotations. For brevity we refer to these states as symmetric vortices. We then solve numerically the GPE for such trial states, for small and for very large values of the nonlinearity ($N\simeq 10^7$). We show how rotation affects the energy of these stationary states and we reach the main result of this section, which is that there are continuous intervals of the ''angular velocity,'' (Ω_m,Ω_{m+1}), in which the m-charged symmetric vortex has less energy than other states of *well defined vorticity*.

In Sec. IV we address the question of the stability of the symmetric states that we introduced in our thesis. We start by describing the three types of stability: *energetic* stability, a state is a local minimum of the energy functional; *Lyapunov* stability, slight perturbations do not destroy the original state; and *linear* stability, Lyapunov stability in the linearized equations. We show the physical implications of each concept and recall how they relate to each other. We next obtain the Bogoliubov equations as the result of linearizing the GPE. We discuss the implications that their proper functions and eigenvalues have for the linear and global stability of vortices and derive several analytic results regarding this question. Finally, in Sec. IV D we collect the most important concepts and propose a numerical algorithm for studying the stability of stationary states of the GPE. This algorithm is applied to the $m=1$ and $m=2$ unperturbed vortex states in stationary traps. It is found that the $m=1$ and $m=2$ vortices are only energetically unstable, which means that the lifetime of both configurations is only limited by dissipation. Further study reveals that rotation can only stabilize the unit charge vortex line if the angular speed is in a suitable range which is almost coincident with (Ω_1,Ω_2). Outside of this range, $\Omega_2<\Omega<\Omega_c$, the minimum of the energy functional is not an eigenstate of the L_z operator—in other words, it is *not symmetric under rotations*—and thus our initial thesis is refuted. These results are complemented by numerical simulations of the evolution of perturbed symmetric vortices that seem to indicate that the $m=1$ and $m=2$ vortices are Lyapunov stable even when they are not minima of the energy functional. In Sec. V we summarize our work and discuss their implications.

II. THE MODEL

For very small temperatures and small densities, the condensate can be accurately modeled by the Gross-Pitaevskii equation (GPE) [3,4]. We will always refer to an axially symmetric trap with a term that accounts for rotation around the Z axis and which may be generated by imposing a suitable weak magnetic field over the trapping potential. The form of the equation is

$$i\hbar\frac{\partial\psi}{\partial t}=-\frac{\hbar^2}{2m}\triangle\psi+\frac{1}{2}m\omega^2(\gamma^2r^2+z^2)\psi + U_0N|\psi|^2\psi+\tilde{\Omega}L_z\psi. \quad (1)$$

Here N is the number of atoms in the gas while $U_0=4\pi\hbar^2a/m$ characterizes the interaction and is defined in terms of the ground-state scattering length, a. By introducing both parameters in the equation, we can impose the following normalization on ψ:

$$\int|\psi|^2d^3x=1. \quad (2)$$

It is convenient to express Eq. (1) in a natural set of units, which for our problem is built up from two scales: the size of the trap (measured by the width of the linear ground state), $a_0=\sqrt{\hbar/m\omega}$, and its period, $\tau=1/\omega$. With these definitions the equation simplifies to

$$i\frac{\partial\psi}{\partial t}=\left[-\frac{1}{2}\triangle+i\Omega\frac{\partial}{\partial\theta}+\frac{1}{2}(\gamma^2r^2+z^2)+U|\psi|^2\right]\psi, \quad (3)$$

while maintaining the normalization (2). Unless otherwise stated, we will use this adimensionalization in all figures throughout the paper.

The new parameters, $\Omega=\hbar\tilde{\Omega}$ and $U=4\pi Na/a_0$, represent the ''angular speed'' of the trap and the adimensionalized interaction strength, respectively. For stability reasons (see below), Ω will be of the order of magnitude of or smaller than the radial strength of the trapping, γ. The interaction, U, will take values from 0 to 6×10^4, which for condensates of rubidium and sodium implies a minimum of 10^6 and a maximum of 10^7 atoms (this is in the range of current and projected experiments). The shape of the trap is dictated by the geometry factor, γ, and in this work it will typically take two possible values: $\gamma=1$ for a spherically symmetric trap, and $\gamma=2$ for an axially symmetric, elongated trap.

A stationary solution of Eq. (3) will be of the form $\psi(\vec{x},t)=e^{-i\mu t}\phi(\vec{x})$ [25], where μ may be interpreted both as a frequency and as a chemical potential,

$$\mu\phi=\left[-\frac{1}{2}\triangle+i\Omega\frac{\partial}{\partial\theta}+\frac{1}{2}(\gamma^2r^2+z^2)+U|\phi|^2\right]\phi. \quad (4)$$

Any solution of Eq. (3) has an energy *per* particle which is given by the functional

$$E(\psi,N)=\int\left(\frac{1}{2}|\nabla\psi|^2-i\Omega\bar{\psi}\partial_\theta\psi\right) + \int\left[\frac{1}{2}(\gamma^2r^2+z^2+U|\psi|^2)|\psi|^2\right]. \quad (5)$$

For a stationary solution it becomes

$$E(\psi,N)=\mu-\frac{U}{2}\int|\phi|^4. \quad (6)$$

The stationary solutions of Eq. (3) may also be regarded as the critical points of

$$\mathcal{L}_\mu = E(\psi,N) - \mu \int |\psi|^2 \tag{7}$$

subject to the constraint of Eq. (2). In that case μ has a third interpretation: it is the Lagrange multiplier of the norm.

III. STATIONARY VORTEX STATES

A. Symmetric vortex states

Since the model which is presented in Eq. (3) has at least axial symmetry and since we are interested in single vortex solutions to the GPE, it is tempting to think that the relevant stationary states of Eq. (3) must also be eigenstates of the L_z operator. We will put forward the thesis that the ground state of Eq. (3) is an eigenstate of L_z. Our purpose in this work is to find these states, to study their stability, and finally to confirm or refute our thesis.

In other words, we are imposing an ansatz for the wave functions that has the form $\psi(r,z,\theta,t) = e^{-i\mu t} e^{im\theta} \phi(r,z)$, and in this section we will search the unit norm functions $\phi_\mu^{(m)}(r,z)$ and real numbers μ, which are solutions of

$$\left[-\frac{1}{2}\triangle - m\Omega + \frac{1}{2}(\gamma^2 r^2 + z^2) + U|\phi_\mu^{(m)}|^2 - \mu \right] \phi_\mu^{(m)} = 0. \tag{8}$$

Our treatment of these equations and of those that we will find throughout this work will be fully three-dimensional, and no spurious conditions (e.g., periodicity) will be imposed on the boundaries. We want to obtain at least the lowest energy state for each value of the vorticity, m. Also the dependency of the spectrum with respect to the nonlinearity and the angular velocity, Ω, is interesting since it will tell us whether the vortex-line states may ever become energetically favorable.

B. Numerical search of stationary states

Due to the nonlinear nature of the problem that we want to solve [Eq. (8)], there are not many analytical tools available. The most common (and maybe the easiest) approach to the problem is to discretize the spatial part and to perform evolution in imaginary time while trying to preserve the normalization, a method which is related to the steepest-descent technique. The precision of the solution depends on the type of the spatial discretization—finite differences (used, for example, in Refs. [20,26]) or spectral methods (such as the one used in Ref. [28]). However, these common methods, such as finite differences [20] and similar spectral methods [21], have up to date reached a maximum value of the interaction coefficient of $U = 10^3$, which is well below the values that can be obtained in experiments. The imaginary time evolution also has serious convergence problems which limit its applicability when $\Omega \neq 0$.

We will present here an approximation technique for these problems. Mathematically speaking, our technique is a Galerkin-type method in which one performs the expansion of the unknown using a complete orthonormal basis of the Hilbert subspace under consideration. For convenience we have used the basis of eigenstates of the harmonic oscillator with fixed vorticity. With that basis our stationary solution is expressed as

$$\psi_\mu^{(m)}(\vec{x},t) = e^{-i\mu t} e^{im\theta} \sum_n c_n P_n^{(m)}(r,z). \tag{9}$$

Here the single index, n, denotes two quantum numbers, (n_z,n_r), that describe the axial and radial degrees of freedom, and $P_n^{(m)}$ is a product of a Hermite polynomial, a Laguerre polynomial, and a Gaussian,

$$P_n^{(m)} = C_n H_{n_z}(z) L_{n_r}(\rho^2) r^m e^{im\theta} e^{-(\rho^2+z^2)/2}, \tag{10a}$$

$$C = \sqrt{\frac{1}{\sqrt{\gamma}\sqrt{\pi} 2^{n_z} n_z!}} \sqrt{\frac{n_r!}{\pi (n_r+m)!}}, \tag{10b}$$

with $\rho = r/\sqrt{\gamma}$

Next, following the same convention about the indices, we have introduced this expansion into Eq. (8) to obtain

$$(E_i^{(m)} - \Omega m - \mu) c_i + U \sum_{jkl} A_{ijkl}^{(m)} \overline{c_j} c_k c_l = 0. \tag{11}$$

Here $E_i^{(m)}$ is the harmonic-oscillator energy of the mode $P_i^{(m)}$, and the tensor $A_{ijkl}^{(m)}$ has the following definition:

$$A_{ijkl}^{(m)} = 2\pi \int \overline{P_i^{(m)}} \overline{P_j^{(m)}} P_k^{(m)} P_l^{(m)} dr dz. \tag{12}$$

Since the $P_i^{(m)}$ are products of known polynomials by exponentials, it could be possible, in principle, to evaluate the tensor exactly with a Gaussian quadrature formula of the appropriate order. This approach was used in Ref. [19] for the three-dimensional case. However, when one wishes to use a large number of modes (which in our case is of about 1600 for each value of m) to achieve large nonlinearities, the search of the quadrature points becomes more difficult than performing a stable integration by means of some other methods, of which the simplest accurate one is Simpson's rule [27].

Once we fix all of the constants, $E_i^{(m)}$, $A_{ijkl}^{(m)}$, μ, and a guess for the solution, it is feasible to solve Eq. (11) iteratively, e.g., by Newton's method [27]. However, it is wiser to perform two simplifications before implementing the algorithm. The first one is that all of the eigenfunctions, $P_n^{(m)}$, can be made real and thus we can impose the coefficients in the expansion, c_n, to also be real.

The second optimization is that, thanks to the symmetry of the problem, the ground state of Eq. (4) has a well defined positive parity. This allows us to eliminate redundant modes [32], saving memory and reaching higher energies and nonlinearities which otherwise would be computationally hard to attain. On the other hand, we have always checked that this method produced the same results as the complete one for a selected and significant set of values of the parameters.

Finally, it is important to note that the tensor of Eq. (12) is indeed a product of two smaller tensors which can be calculated by integrating on the z and r variables, respectively [19]. This decomposition is most important when working

with a large number of modes, because then the size of $A^{(m)}_{ijkl}$ becomes extremely large (i.e., 1600^4 elements for 1600 modes).

Concerning the evaluation of polynomials of a very high degree as the ones involved in our computations, we must say that it is not a simple task. This is especially difficult for intermediate values of the spatial variables since in that range there are a lot of terms with opposite signs and similar magnitude, and the cancellations induce numerical instabilities. The usual procedure to avoid this difficulty is to use Horner's method [27] to evaluate the polynomial, which is comparable to using fast Fourier transform (FFT) techniques, but in our case this is not enough and the evaluation of the polynomials could only be done using recursive formulas which are specific to the Hermite and Laguerre basis.

We remark that the election of this spectral technique was largely influenced by the need for reaching high nonlinearities which are not achievable using the other approaches. Further details on the numerical technique as well as convergence proofs will be given elsewhere [29].

C. Results for stationary traps

By using the preceding technique, we have searched the lowest states $(n_z, n_r = 0)$ for each branch of the spectrum with a different vorticity, $m = 0, \ldots, 6$. This was performed for two geometries corresponding to $\gamma = 1$ (spherically symmetric trap) and $\gamma = 2$ (cigar shape trap), of a stationary trap, $\Omega = 0$, while varying the intensity of the interaction from 0 to approximately 50 000. The results of this study are plotted in Fig. 1.

Remarkably, in the absence of rotation, and up from the lowest states, both the spectrum and the energies can be fitted to a simple formula,

$$\mu_{0m}(N) \simeq \mu_{00}(N) + \omega_{\mathrm{eff}}(N) m, \tag{13a}$$

$$E_{0m}(N) \simeq E_{00}(N) + \tilde{\omega}_{\mathrm{eff}}(N) m. \tag{13b}$$

The first term is the chemical potential of the $m = 0$ ground state and it is irrelevant for the dynamics. Using the Thomas-Fermi limit, one can show that it grows proportionally to $\mu \propto N^{2/5}$, a behavior which is approximately reflected in the numerical results [Fig. 1(c)].

The second term is much more relevant to the evolution of the condensate. It grows linearly, as the energy levels of a linear harmonic oscillator with an effective frequency, $\omega_{\mathrm{eff}}(N)$, that decreases with the interaction. The fact that the highest levels of the spectrum of μ remain equispaced even for large interactions is the reason why the condensate exhibits an exponentially divergent response to the parametric perturbation of the trap frequencies, as it is shown in Refs. [30] and [31].

D. Results for rotating traps

Now we want to study the stationary solutions in the presence of rotation. For $\Omega \neq 0$, the solutions with definite vorticity remain the same, while their chemical potential and energy suffer a shift that depends on the vorticity of the state,

$$E_{nm}(U, \Omega) = E_{nm}(U, 0) - m\Omega. \tag{14}$$

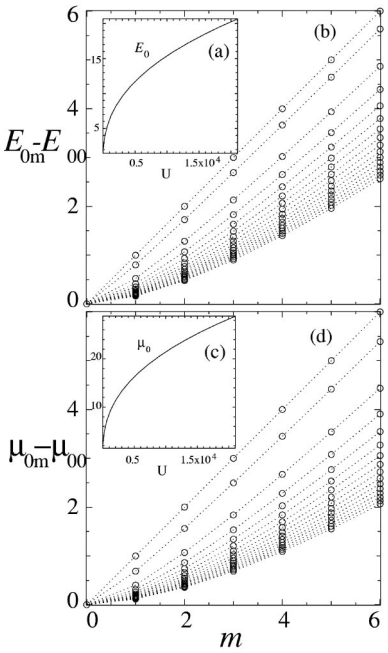

FIG. 1. Plots (a) and (c) show the ground-state energy, E_{00}, and chemical potential, $\mu_{00}(U)$, dependence on the interaction strength. Plots (b) and (d) show the chemical potential and the energy of the lowest state for each vorticity, always relative to value the ground state. The interaction values range from $U = 0$ (upper diagonal) to $U = 50\,000$ (lowest diagonal). All calculations shown correspond to the spherically symmetric trap, $\gamma = 1$, and all quantities have been adimensionalized using the rules of Sec. II.

This shift gives rise to an ample phenomenology, which is pictured in Fig. 2. First, we see that the degeneracy with respect to m is broken. The only other possible degeneracy that remains is with respect to the r and z variables, but it disappears in the case without spherical symmetry, $\gamma \neq 1$.

Second, the $m = 1,2,3, \ldots$ branches of the spectrum become a minimum of the energy functional with respect to other branches for continuous intervals of the angular velocity (Ω_m, Ω_{m+1}). We will refer to these values of the angular velocity as *stabilizing frequencies*. They are given by the simple formula

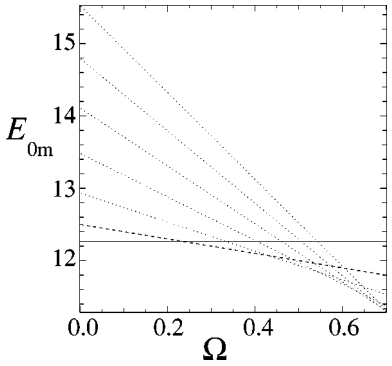

FIG. 2. Dependence of the energy levels on Ω, $E_{0m}(U, \Omega)$, for a fixed value of the interaction strength, $U \simeq 8000$, and a spherically symmetric trap, $\gamma = 1$. The horizontal line represents the vortex-free state, $m = 0$, the dashed line the $m = 1$ vortex state, and the dotted lines other multicharged vortex states.

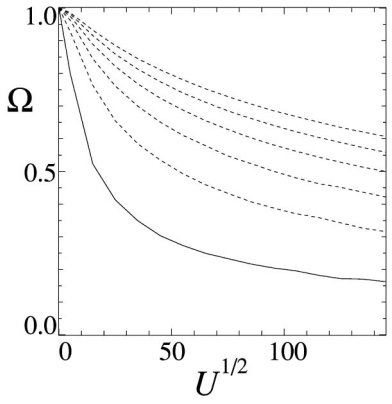

FIG. 3. Frequency of stabilization of the vortex states in a spherically symmetric trap, $\gamma=1$, as a function of the nonlinearity. The lines are arranged in order of increasing vorticity, from $m=1$ (solid line) to $m=6$ (dashed line on the top).

$$\Omega_m = E_{0,m+1} - E_{0m}. \tag{15}$$

However, we cannot assure at this point that on those intervals the mth vortex state becomes a global minimum. Indeed, in Sec. IV we will be able to prove that only the $m=1$ vortex lines achieve the status of local minima. It still remains an open question to provide an analytic proof of this fact.

Third, even though the separation between the $m=0$ and $m=1$ states becomes very narrow for large interactions, the stabilizing frequency Ω_1 only approaches zero asymptotically with U. As a consequence, $m=1$ states are never a global minimum of the energy in a stationary trap, a fact that can be checked by just inspecting the energy functional.

And finally, there is a critical value of Ω for which the energy functional becomes unbounded by below (see Fig. 3). In the linear case, this critical value of the frequency, Ω_c, is such that all of the ground states for each value of the vorticity have the same energy. Here we can define it as a limit

$$\Omega_c(U) = \lim_{n\to\infty} \Omega_n(U). \tag{16}$$

Using Eqs. (16) and a fit such as the one in Eq. (13), one finds that Ω_c coincides with the separation between energy levels for large values of the vorticity and is always smaller than the critical frequency of the linear case,

$$\Omega_c = \omega_{\mathrm{eff}}(U). \tag{17}$$

IV. STABILITY OF STATIONARY STATES

A. Types of stability

In the preceding section we obtained stationary solutions of the mean-field model for the Bose-Einstein condensate, all of which had a well defined value of the third component of the angular momentum operator. We named those states symmetric vortices or just vortices. In this section we want to study the stability of these solutions according to several criteria.

From a mathematical point of view, there are many definitions of stability. Here we will concentrate on three of them that are useful for our system and have a clear physical interpretation. First, we have the most intuitive definition, which is that of *energetic stability*. We say that a state of a system is locally or globally energetically stable when it is a local or global minimum of the energy functional, respectively. Second, we say that a state is *Lyapunov or dynamically stable* when for sufficiently small perturbations the system remains arbitrarily close to the original state for all times. Finally, we will use the concept of *linear (dynamical) stability*, which can be defined as the stability of the system for infinitesimal perturbations. An equivalent definition of the later concept is the Lyapunov stability of the linearized evolution equations around the stationary state.

These three concepts are not equivalent. It is well known, however, that *energetic stability implies Lyapunov stability* and *Lyapunov stability implies linear stability*. Intuitively, the Lyapunov stability is the closest one to what we usually think of as ''stability'' and it would be desirable to characterize the dynamical stability of a state. Energetic stability should ideally qualify how the system behaves when dissipation is introduced in the system; it is also a sufficiency condition for dynamical stability and a necessary condition for a state to be a ground state. And finally, a study of linear stability tells us about the absence of Lyapunov or energetic stability and about the behavior of the system for sufficiently short times.

With these considerations in mind, we can think of indirectly studying the question of Lyapunov stability both from a linear and a global point of view. We will explain this statement in the following subsections.

B. The linear stability equations

Since we are interested in linear stability, let us begin our study from the adimensionalized Gross-Pitaevskii equation (3) and expand the condensate wave function around a stationary solution with a fixed vorticity,

$$\Psi(r,z,\theta,t) = \psi_0 + \epsilon\psi_1 = [f(r,z)e^{im\theta} + \epsilon\alpha(r,z,\theta,t)]e^{-i\mu(\Omega)t}. \tag{18}$$

We insert this expansion into Eq. (3) and truncate the equations up to $O(\epsilon^1)$, thus obtaining

$$i\partial_t\alpha = (H_0 + i\Omega\partial_\theta + 2Uf^2)\alpha + Uf^2e^{-2im\theta}\overline{\alpha}, \tag{19a}$$

$$-i\partial_t\overline{\alpha} = (H_0 - i\Omega\partial_\theta + 2Uf^2)\overline{\alpha} + Uf^2e^{2im\theta}\alpha, \tag{19b}$$

with $H_0 = -\frac{1}{2}\triangle + \frac{1}{2}(\gamma^2r^2 + z^2) - \mu(\Omega)$. We can also write this equation in a more compact form,

$$i\frac{\partial}{\partial t}\vec{W} = \sigma_z\mathcal{H}(\Omega)\vec{W} = \mathcal{B}(\Omega)\vec{W}, \tag{20}$$

by using the following definitions:

$$\vec{W} = \begin{pmatrix} \alpha \\ \overline{\alpha} \end{pmatrix}, \tag{21a}$$

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{21b}$$

$$\mathcal{H}(\Omega) = H_0 + \begin{pmatrix} i\Omega\partial_\theta + 2Uf^2 & Uf^2e^{-2im\theta} \\ Uf^2e^{2im\theta} & -i\Omega\partial_\theta + 2Uf^2 \end{pmatrix}. \tag{21c}$$

To characterize the linear stability of a state, we are interested in the dynamics that is involved in Eq. (20). The simplest way to learn about it is to find a suitable basis in which Eq. (20) can be diagonalized. In other words, we want a set of vectors, $\vec{W}_k^t=(u_k(r),v_k(r))$, such that

$$\lambda_k\vec{W}_k=\mathcal{B}\vec{W}_k. \tag{22}$$

If $\mathcal{B}$ has such a diagonal Jordan form, then it follows that a perturbation evolves simply as

$$\vec{W}=\sum c_k e^{i\lambda t}\vec{W}_k, \tag{23}$$

$$\alpha(\vec{r},t)=\sum c_k e^{i\lambda t}u_k(\vec{r},t), \tag{24}$$

On the other hand, the lack of a diagonal form, or the existence of complex eigenvalues, apparently leads to instability since we have modes that grow polynomially in time. Thus a study of the eigenfunctions of the linearized equations gives us all the information we need about linear stability.

We will also see that this diagonalization is related to the behavior of other properties of a perturbed state in general and to energetic stability in particular. Associated with Eq. (20) there is an energy functional,

$$E_2(\alpha)=\int 2\overline{\alpha}H_0\alpha+\psi_0^2\overline{\alpha}^2+\overline{\psi}_0^2\alpha^2+4|\psi_0|^2\alpha\overline{\alpha}, \tag{25}$$

and a constrained energy functional,

$$\mathcal{L}_2(\alpha)=E_2(\alpha)-\mu\int|\alpha|^2, \tag{26}$$

which are the $O(\epsilon^2)$ terms in the expansion of Eqs. (6) and (7), i.e., the free energy introduced in the system by the perturbation. If a diagonal Jordan form such as that of Eq. (22) is possible, then the second functional becomes diagonal too,

$$\mathcal{L}_2(\alpha)=\sum|c_k|^2\lambda_k G(\vec{W}_k), \tag{27a}$$

$$G(\vec{W}_k)=\int|u_k|^2-|v_k|^2. \tag{27b}$$

If the stationary state, ψ_0, is a local minimum of the energy subject to the constraint of a fixed norm (2), then $\mathcal{L}_2$ must be positive for all perturbations, which has obvious implications for the eigenvalues and eigenstates.

Combining our knowledge about the linearized equations and linearized functionals, one may find two distinct situations. First, the Bogoliubov operator may have complex eigenvalues or even have a nondiagonal Jordan form. In both cases we customarily speak of *linear dynamical instability* because an arbitrarily small perturbation departs from the original state exponentially or polynomially in time. Second, the linearized operator may have only real eigenvalues which should be interpreted as the change of energy in the condensate due to excitations [see Eq. (26)]. If $\lambda>0$, the state under study ψ_0 is a local minimum of the energy functional (5) with respect to this family of perturbations, the $\lambda=0$ case corresponds to the existence of degeneracy in the system, and finally if $\lambda<0$ the system is told to be energetically unstable, i.e., excitations are energetically favorable and the state is not a local minimum of the energy.

When studying the condensate using tools from quantum field theory, one may try a similar procedure [19], which is known as Bogoliubov's theory. In that framework, $\overline{\alpha}$ and α are linear operators in a Fock space and one searches an expansion of these operators in terms of others that diagonalize the energy functional (25) and the evolution equations (20). The resulting equations for the coefficients are known as Bogoliubov's equations and correspond to Eqs. (22) for u_k and v_k. All of the five cases exposed above have the same implications on stability for Eq. (3), which is a partial differential equation for an order parameter, and for the more complete Bogoliubov theory, where the perturbations are regarded as many-body corrections and involve more degrees of freedom.

Finally, we want to comment that energetic instabilities are less ''harmful'' than dynamic ones, as they affect the dynamics only when there is some kind of dissipation that drives the system through the unstable branch. And even then the lifetime of the system could be large if the intensity of the destabilizing mode were small compared to the typical evolution times.

C. Analytic results

Here we present several results on the connection between eigenvalues [Eq. (37)] and destabilizing modes.

1. Lack of exponential instabilities in the Bogoliubov theory

Any eigenvalue λ satisfying Eq. (37) and $G(\vec{W})\neq0$ must be real. Eigenstates with $G(\vec{W})=0$ may involve complex eigenvalues but they are spurious and introduced by the linearization procedure.

This first part is proven simply by projecting the left and right hands of Eq. (37) on $\vec{W}_i^{(n)\dagger}$. Omitting the indices, the result is

$$\lambda_n\int(|u|^2-|v|^2)=\int(\overline{u}_nH^nu+\overline{v}H^{2m-n}v)+\int Uf^2|u+v|^2-\int(n-m)\Omega(|u|^2+|v|^2). \tag{28}$$

The second part is more subtle. To prove it, we must recall that solutions of Eq. (20) are stationary points of the action [30], $S=\int L(t)dt$ corresponding to the following Lagrangian density:

$$L=\int\frac{i}{2}(\alpha\overline{\alpha}_t-\overline{\alpha}\alpha_t)+\mathcal{L}_2(\alpha). \tag{29}$$

Using Eq. (27a), one shows that the modes with $G(\vec{W})=0$ are null modes that do not appear in the linearized Lagrangian, and thus have no influence on the dynamics.

From a mathematical point of view, when there exist complex eigenvalues, one can think of a plateau in the energy functional such that, if we move along the eigenfunc-

tions corresponding to these eigenvalues, the energy change is of order $O(\epsilon^3)$ and thus the linearization procedure, which goes up to $O(\epsilon^2)$, cannot account for the dynamic along those directions.

It is important to keep in mind that this theorem does not grant that $\mathcal{B}_n$ has a Bogoliubov diagonalization. It would be desirable to have an analytic result that solves this question.

2. Sufficient condition for stability

If the linearized Hamiltonian $\mathcal{H}_n$ is positive definite, then $\mathcal{B}_n$ may be diagonalized, all of its eigenvalues are positive real numbers, and there are neither dynamical nor energetic instabilities.

To prove this theorem, one only needs to show that there is a one-to-one correspondence between the eigenfunctions of $\mathcal{H}_n^{1/2}\sigma_z\mathcal{H}_n^{1/2}$ and the eigenfunctions of $\sigma_z\mathcal{H}_n$ so that

$$\mathcal{H}_n^{1/2}\sigma_z\mathcal{H}_n^{1/2}|n\rangle=\lambda|n\rangle, \tag{30}$$

if and only if

$$\sigma_z\mathcal{H}_n\mathcal{H}_n^{(-1/2)}|n\rangle=\lambda\mathcal{H}_n^{(-1/2)}|n\rangle. \tag{31}$$

This implies that the eigenvalue in Eq. (37) must be positive.

3. Stability in stationary traps

In Eq. (37), if $\Omega=0$ and $n>3m$, then the linearized Hamiltonian $\mathcal{H}_n$ is positive, the Bogoliubov operator $\mathcal{B}_n$ can be diagonalized, and it is also positive. Furthermore, if $n>m$, then any real eigenvalue is positive, $\lambda>0$.

The proof has several steps. First, one takes any value of n that satisfies that condition and proves that $H^{2m-n}>H^m$ and $H^n>H^m\geqslant 0$. Second, this fact is used to prove that $\mathcal{H}_{0n}>\mathcal{H}_{0m}$. Third, it is shown that $\mathcal{U}_n$ is positive, which altogether implies $\mathcal{H}_n>0$. The last assertion may be easily checked with the help of Eq. (28).

The preceding two theorems imply that in a stationary trap any mode with negative energy must be comprised in the $(0,-2m),\ldots,(m,m)$ families, and any dynamic instability must lay in $(0,-2m),\ldots,(3m,0)$. Thus we need only diagonalize a finite number of operators to analyze the stability of a vortex state. This result is an extension of the one obtained in Ref. [17], where a sufficient condition for stability is found to be $n^2\geqslant 4m^2$, without taking into account possible complex eigenvalues.

4. Local stability under rotation

In Eq. (37), the operator $\mathcal{B}_n(\Omega)$ exhibits a linear dependence with respect to Ω,

$$\mathcal{B}_n(\Omega)=\mathcal{B}_n(0)-(n-m)\Omega. \tag{32}$$

While the wave functions of the modes are the same as those of the stationary traps, the energies of the excitations suffer also a shift that depends on the vorticity,

$$\lambda(\Omega)=\lambda(0)-(n-m)\Omega. \tag{33}$$

In general, the influence of these shifts has to be checked numerically. It is easy to show, however, that the shift is positive for $n<m$, which means that one can expect to suppress the possibly negative eigenvalues in the range $0<n<m$ if Ω is large enough. Even more, as the shift is a real number, if one were able to demonstrate that there are no dynamical instabilities in the stationary trap, then there would be no dynamical instabilities in the rotating trap.

TABLE I. Relation between the diagonalization of the linearized equations and the linear and global stability of a state.

λ	Linear stability	Global stability
Nondiagonal box	Unstable	Lyapunov unstable
Complex eigenvalue	Undetermined	Undetermined
$\exists\ \lambda<0$	Stable	Energetically unstable
$\lambda>0,\ \forall\ \lambda$	Stable	Energetically stable

D. A numerical algorithm for the study of the stability

Let us collect and simplify what has been exposed in the preceding subsections by formulating the algorithm that we have used to study the stability of the vortex states of Sec. III.

The algorithm must be applied to each symmetric vortex separately. The first step consists in linearizing the evolution equations to obtain

$$i\frac{\partial\vec{W}}{\partial t}=\mathcal{B}\vec{W}. \tag{34}$$

Second, one has to search the Jordan form of the B operator on a suitable finite-dimensional space. In the third step, one must classify the Jordan boxes and eigenvalues according to Table I and obtain the information about the stability. In case of instability, depending on the magnitude of the eigenvalues one can check whether they can be suppressed with an appropriate choice of parameters, namely Ω. The fourth stage of the algorithm consists of checking that the size of the subspace does not influence the results. To ensure the validity of the results, we have checked them with numerical simulations of the evolution of perturbed states.

E. Numerical procedure

It is useful to expand α and $\overline{\alpha}$ into states of fixed vorticity so that the modes are separated into disjoint subspaces,

$$\vec{W}_i^{(n)}=\begin{pmatrix} u_i^{(n)}(r)e^{in\theta} \\ v_i^{(2m-n)}(r)e^{i(2m-n)\theta}\end{pmatrix}. \tag{35}$$

These subspaces are not mixed by the action of the operators of Eq. (21) and we can define their restriction to these subspaces separately as

$$\mathcal{B}_n(\Omega)=\sigma_z\mathcal{H}_n(\Omega), \tag{36a}$$

$$\mathcal{H}_n(\Omega)=\mathcal{H}_{0n}(\Omega)+\mathcal{U}_n, \tag{36b}$$

$$\mathcal{H}_0=\begin{pmatrix} H^n-(n-m)\Omega & \\ & H^{2m-n}-(m-n)\Omega\end{pmatrix}, \tag{36c}$$

$$H^n = -\frac{1}{2}\triangle + \frac{1}{2}(\gamma^2 r^2 + z^2) + \frac{n^2}{2r} + f^2 - \mu(0), \quad (36d)$$

$$\mathcal{U}_n = Uf^2 \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}. \quad (36e)$$

With these definitions the eigenvalue equations (22) become

$$\lambda_k^n \vec{W}_k^{(n)} = \mathcal{B}_n(\Omega)\vec{W}_k^{(n)}, \quad n \geqslant m. \quad (37)$$

If $G(\vec{W}_k^{(n)})>0$, then $(u_k^{(n)}, v_k^{(2m-n)})$ is a Bogoliubov mode with energy $\epsilon = \lambda_k^{(n)}$ and vorticities $(n, 2m-n)$, whereas if $G(\vec{W}_k^{(n)})<0$, then the excitation is $(v_k^{(2m-n)}, u_k^{(n)})$ with energy $\epsilon = -\lambda_k^{(n)}$. As a rule of thumb, to place all the relevant information in the eigenvalue, the u function must always be the one with the largest contribution. This is formally stated in $G(\vec{W})>0$. In the following, we will refer to these branches of the spectrum by the pairs of quantum numbers $(n, 2m-n)$ and $(2m-n, n)$, respectively.

We have discretized Eq. (37) in a basis which is the Cartesian product of twice the one we used to solve the stationary GPE. To be more precise, using the notation of Sec. III the expansion is as follows:

$$\vec{W}_i^{(n)} = \sum_k a_k \begin{pmatrix} P_{kn} \\ 0 \end{pmatrix} + \sum b_l \begin{pmatrix} 0 \\ P_{l,2m-n} \end{pmatrix}. \quad (38)$$

In this basis, the operator $\mathcal{H}_{0n}$ is diagonal, while the operator $\mathcal{U}$ must be evaluated, either by means of integrals of the wave function itself in position representation or by using a tensor which is larger but equivalent to the one in Eq. (12). In any case, the equations are always linear and so the study of the Bogoliubov spectrum consists in building and diagonalizing a large real matrix.

Even though the procedure is quite simple, the matrices that one must build, especially in the case of strong interaction, are very large and tend to exhaust computational resources. To reach large values of the nonlinearity, we had to work in a subspace of states with even parity with respect to the Z axis. This way we could find the excitations with lowest energy for different vorticities at the cost of missing those with odd parity, which are more energetic anyway [32].

F. Numerical results

Now that stationary vortex states have been found, as discussed in Sec. III, we are going to present now our stability results obtained with the previously described algorithm.

1. Stability of the m=1 vortex line in a stationary trap

In this case one has to study a single operator, $\mathcal{B}_0$, to know whether the state is stable. This calculation provides a branch of the spectrum of excitations that is denoted by the quantum numbers (0,2) and (2,0). We performed the same procedure for a wide range of nonlinearities in the absence of rotation, $\Omega = 0$, and the first conclusion is that the Bogoliubov operator has a diagonal Jordan with real eigenvalues.

In Fig. 4 we show a selected set of the eigenvalues of the Bogoliubov operator, both for a spherically symmetric trap and an elongated trap. In those pictures several things are clear. First, there are two constant eigenvalues $\lambda = 1$, which correspond to oscillations of the vortex line along the Z axis. Second, there is a neutral mode $\lambda = 0$ for the spherically symmetric trap, which corresponds to the rotation symmetry of the condensate around an axis on the XY plane. The symmetry and the mode disappear when $\gamma = 2$ (see Fig. 4). Finally, there is at least one negative eigenvalue $\mu < 0$ (more in the case of elongated traps), which is responsible for the energetic destabilization of the system. The largest contribution to this destabilizing mode corresponds to a wave function that is captured in the vortex line and has zero vorticity, i.e., it is a *core* mode (see Fig. 5), as was qualitatively predicted by Rokhsar in Ref. [16].

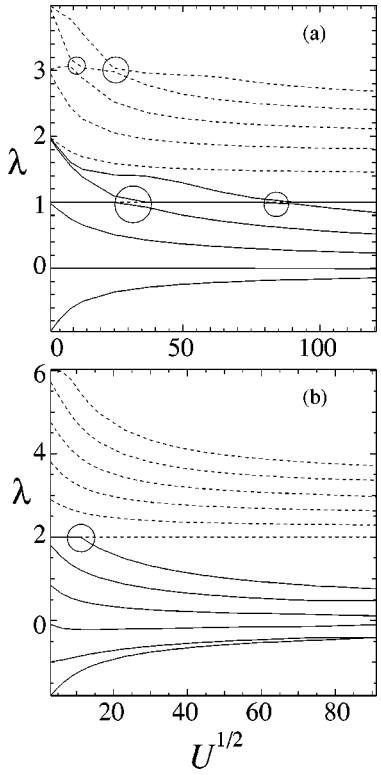

FIG. 4. Lowest eigenvalues of the Bogoliubov operator $\mathcal{B}_0$ for the $m=1$ unperturbed state in (a) a spherically symmetric trap, $\gamma = 1$, and (b) an axially symmetric trap, $\gamma = 2$. The solid lines represent modes with quantum numbers (0,2) and the dashed lines represent modes of the (2,0) family. Crossing of levels is signaled with circles as a visual aid.

We must remark that the number of unstable modes increases with the geometry factor—the more elongated the trap is, the easier it is to transfer energy from the vortex to the core plus longitudinal excitations. In other words, while for spherical and ''pancake'' traps ($\gamma \leqslant 1$) there is only one negative eigenvalue which corresponds to an excitation with a vorticity different from the unperturbed function, for elongated traps ($\gamma > 1$) we still have that mode plus some others which represent excitations along the Z axis. As a consequence, if the experiment is subject to dissipation and these unstable modes play a significant role in the dynamics, then the more elongated the trap is, the less stable the vortex will be.

In Fig. 6 we show the lowest eigenvalues of the families $(-1,3)$, $(1,1)$, $(0,2)$, $(2,0)$, and $(-2,-4)$, that is, excita-

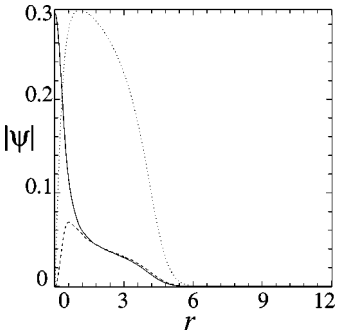

FIG. 5. Shape of the destabilizing mode. We show both the original solution (dotted line), the largest contribution u (dashed line), and the smallest contribution v (solid line). Functions have been rescaled to aid visualization.

tions where the main contribution is an eigenstate of L_z with eigenvalues $m=0,\pm 1,\pm 2$. In those pictures one sees that excitations with the same vorticity but opposite sign also have different energy, a phenomenon which is solely due to the interaction.

2. Stability of m=1 vortex lines in rotating traps

It was already proved [Eq. (32)] that as the effect of rotation is gradually turned on, the modes with $n<m$ and with $n>m$ are shifted up and down in the spectrum, respectively. A natural question concerns whether this shift is enough to stabilize the vortex states. We prove using numerical experiments that this is the case for our system.

It can be seen in Fig. 7 that the negative eigenvalue is slightly smaller than the stabilizing frequency, $|\lambda_0|<\Omega_1$, which implies that for $|\lambda_0|<\Omega<\Omega_c$ the energetically unstable branch with vorticity $m=0$ disappears. Also the eigenvalues of $\mathcal{B}_n$ for $n>m$ are found to be larger than $(n-m)\Omega_1$. Thus, all the operators $\mathcal{B}_n$ are positive at least in the interval (Ω_1,Ω_2) and consequently the vortex with unit charge is a local minimum of the energy functional. Indeed, there is a small interval $(|\lambda_0|,\Omega_1)$ in which the vortex is stable and there is a local minimum of the energy functional, while the ground state has no vorticity at all.

Finally, the shifts are always real, which implies that the $\mathcal{B}_n$ operators remain diagonalizable with real eigenvalues and without dynamical instabilities.

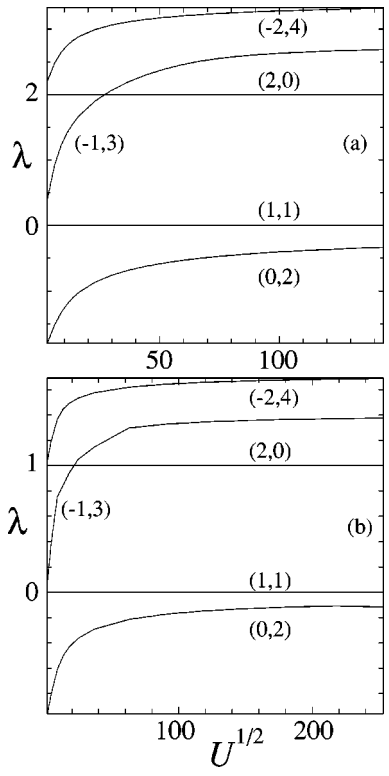

FIG. 6. Excitation energy of the lowest Bogoliubov modes for an unperturbed state with $m=1$. The vorticities of each mode are written close to its corresponding line. Plot (a) corresponds to $\gamma=1$, and (b) to $\gamma=2$.

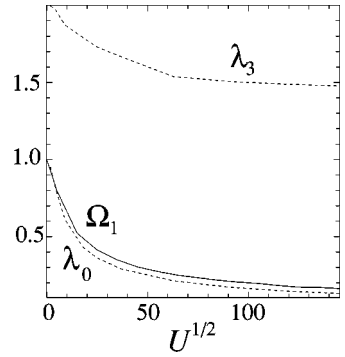

FIG. 7. Ω_1 (solid line), $-\lambda_0$ (lower dashed line), and λ_3 (upper dashed line) for a spherically symmetric trap, $\gamma=1$.

3. Stability of the m=2 vortex line

Another interesting configuration is the $m=2$ multicharged vortex line. Here one suspects that a configuration with several vortices of unit charge has less energy than a single multicharged vortex, under all circumstances. In other words, they must be always energetically unstable.

This intuitive perception is confirmed by the numerical analysis. First the diagonalization of $\mathcal{B}_1$ reveals that this operator has at least one negative eigenvalue, while $\mathcal{B}_0$ has negative eigenvalues and a pair of complex eigenvalues that, as we saw above, do not participate in the dynamics and must be discarded. Regarding the negative eigenvalues, they do not decrease with the nonlinearity, but are always larger in absolute value than their linear limits. This implies that there are always negative eigenvalues which cannot be suppressed with any rotation below the critical value, $\Omega_2<\Omega<\Omega_c\leqslant\gamma$.

The immediate consequence of this linear stability analyses is that, since the linearization of the energy (25) is not positive, the $m=2$ vortex line is never a local minimum of the energy. This is true even for the parameter interval, (Ω_2,Ω_3), in which it has less energy than the rest of the stationary symmetric vortices. If the $m=2$ ground state is not a minimum, and the other symmetric states have more energy, we can conclude that the minimum of the energy functional in the rotating trap with $\Omega\in(\Omega_2,\Omega_3)$ must be a state which is not symmetric with respect to rotations, as it was proposed in Ref. [24] for small nonlinearities. A similar analysis can be performed for the stationary states with $m=3,4,\ldots$, which extends this result to larger rotation frequencies that are all below the critical one.

G. Lyapunov stability

As we saw above, a solution of Eq. (3) is Lyapunov stable when every slightly perturbed solution remains close throughout the unperturbed one. It is very difficult to study Lyapunov stability of stationary solutions of Eq. (3) in a rigorous way, a point which deserves further investigation. Here we have performed an ''empirical'' study of the Lyapunov stability of the stationary solutions with $m=1$ and $m=2$ by simulating numerically how they evolve for small perturbations and long times. The simulation was performed with a three-dimensional split-step pseudospectral method like that of Ref. [30], using an $80\times80\times80$ points grid to study both the $\gamma=1$ and $\gamma=2$ problems.

The main result of this complementary work is that both the unit charge vortex line and the multicharged vortex line are stable to perturbations which involve the destabilizing modes as defined by Eq. (37). For example, one may try to add a small contribution (0.5%) of a core mode to the $m=2$ vortex, with the result that the vortex line is split into two unit charge vortex lines which rotate but remain close to the origin. We must remark that, although these simulations only work for finite times which are dictated by the precision of the scheme and the computational resources, these times are typically 20 or 30 periods of the trap, which is much larger than any of the magnitudes that one may address theoretically to the destabilization process, i.e., the negative or complex eigenvalues of Eq. (37).

In the end, what these types of simulations reveal is that the $m=1$ and $m=2$ stationary states are energetically unstable, but this has no influence on the dynamic unless some other ''mixing'' or dissipative terms participate in the model.

V. CONCLUSIONS

We have studied the vortex solutions of a dilute, nonuniform Bose condensed gas as modeled by the Gross-Pitaevskii equation (3), both in a stationary, axially symmetric trap and subject to rotation (or a uniform magnetic field).

First, we have searched solutions of Eq. (4) that have the lowest energy and which are also eigenstates of the third component of the angular momentum operator, $\psi(r,z,\theta)=f(r,z)e^{im\theta}$, in stationary and rotating traps using different values of the nonlinear coefficient ranging from small to very large values. It has been found that a nonzero angular speed is required in order to turn a vortex line state into a minimum of the energy functional with respect to other states of well-defined vorticity.

Next, we have studied the stability of these stationary solutions of the GPE. We have derived a set of coupled equations that account for both the linearization of the GPE around a stationary solution and Bogoliubov's corrections to the mean-field theory that describes the condensate. It has been proved that the problem may not exhibit dynamical instabilities of an exponential nature. In addition, several other theorems have been proved that describe the phenomenology associated with the relevant modes.

The perturbative equations have been solved numerically for stationary states having $m=1$ and $m=2$ vorticities. In both cases it has been found that the only instability is of an energetic nature, being limited to a small number of modes whose nature was already predicted qualitatively in [16].

For the vortex with unit charge, we have found that this instability may be suppressed by rotating the trap at a suitable speed, and even when the trap is stationary it is expected that it plays no significant role in the dynamics, unless there is enough dissipation to take the system through the unstable branch. On the other hand, the linear stability analysis for the $m=2$ multicharged vortex reveals that the energetic instability may never be suppressed and that this configuration is never a minimum of the energy functional, even though its lifetime is, once more, only conditioned by possible dissipation.

The last and probably most important conclusion of this work is that in the rotating trap, and for $\Omega>\Omega_2$, the state of minimum energy is not an eigenstate of the L_z operator, and thus it is not symmetric with respect to rotations. A similar result was predicted qualitatively in Ref. [24] by means of a minimization procedure that is only justified in the limit of very small U. Our proof remains valid for the entire range of nonlinearities used here.

From an experimental point of view, this work has several implications. First, vortex lines with unit charge may be produced by rotating the trap at a suitable speed and then cooling the gas. Second, once rotation is removed, these vortices will survive for a long time if dissipation is small. Third, the symmetric multicharged vortices are not minima of the energy functional and thus it will be difficult to generate them by means of cooling a rotating gas. And finally, if these multicharged vortices are generated by some other means, then we can expect that their lifetime will only depend on the intensity of dissipation, whose effect is to take the system either to the $m=0$ ground state if $\Omega<\Omega_1$, to the unit charge vortex line state if $\Omega<\Omega_2$, or to a symmetryless multicharged state if $\Omega_2>\Omega$ (a phenomenon that is known as splitting in the literature).

The numerical results obtained have been possible due to the use of a powerful Galerkin spectral method that has been optimized to allow for the consideration of thousands of modes, which is a step forward with respect to the previous analysis.

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