Dynamic stability of a doubly quantized vortex in a three-dimensional condensate

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Abstract

The Bogoliubov equations are solved for a three-dimensional Bose-Einstein condensate containing a doubly quantized vortex, trapped in a harmonic potential. Complex frequencies, signifying dynamical instability, are found for certain ranges of parameter values. The existence of alternating windows of stability and instability, respectively, is explained qualitatively and quantitatively using variational calculus and direct numerical solution. It is seen that the windows of stability are much smaller for a cigar shaped condensate than for an oblate one, which explains the findings of recent experiments.

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I. INTRODUCTION

One of the hallmarks of superfluid flow is the quantization of fluid circulation. Its manifestation through the formation of quantized vortices is a long studied subject in superconductors, superfluid Helium and trapped atomic gases [1]. Although a vortex can in principle carry any number of circulation quanta, it is well known that in an infinite homogeneous system, only singly quantized vortices are energetically allowed, since a vortex with quantum number larger than unity, frequently called a giant vortex, has higher energy than the corresponding number of separated vortices with single quanta, while carrying the same angular momentum.

For Bose-Einstein condensates trapped in magnetic potentials, the situation is more complicated since the size of a vortex core can be comparable to the total system size. Still, it is an accidental fact that quantum numbers larger than unity are energetically unfavorable in Bose-Einstein condensates in parabolic potentials, just as in the homogeneous case. This result hinges on the fact that in the noninteracting limit, the lowest energy levels with a given angular momentum are vastly degenerate; interactions lift the degeneracy and favor a state with a diluted density profile, which is a lattice of singly quantized vortices. The situation is different if the trapping potential is steeper than harmonic, in which case giant vortices are energetically favorable in the limit of weak interactions [2].

The related but separate issue of *dynamical* stability of doubly quantized vortices has become especially relevant lately since the problem can be readily probed by experimental means [3]. Theoretically, it is known that in the two-dimensional limit such a vortex is dynamically unstable towards splitting into two only in certain windows of parameter space, when the interaction strength lies within certain intervals [4]. These intervals have been shown to be bounded by zeros of eigenvalues for the corresponding static stability problem [5]. However, the situation is entirely different in three dimensions: in the strongly cigar shaped limit, instabilities are expected to lie densely in phase space, because of the closely spaced energy levels in the third direction [6, 7].

In this paper, we perform a systematic study of the Bogoliubov excitations in two- and three-dimensional condensates containing a doubly quantized vortex. The paper is organized as follows. In Sec. II we discuss the equations and the structure of the stability problem. In Sec. III we address the the two-dimensional problem and show how the observed parameter dependence can be understood and approximated analytically. Section IV contains an overview of the numerical results for the three-dimensional condensate. In Sec. V we discuss in greater detail the limit of a cigar shaped condensate. Section VI relates the present results to experimental findings. We calculate the instability regions for an anharmonic trap in section VII, to investigate the stability in a more general case. Finally, in Sec. VIII we summarize and conclude.

II. STABILITY PROBLEM FOR A CONDENSED BOSE GAS

The system under study is a Bose-condensed atomic gas that is trapped in a cylindrically symmetric harmonic potential. At zero temperature in the dilute limit it is described by a condensate wavefunction $\Psi(r, \theta, z, t)$ that obeys the Gross-Pitaevskii equation

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) + U_0|\Psi|^2\right]\Psi = \mu\Psi. \tag{1}$$

The eigenvalue μ is the chemical potential, which ensures that the wavefunction Ψ is normalized to the number of atoms N. The trapping potential is assumed to be of the form

$$V(\mathbf{r}) = \frac{m\omega_\perp^2}{2}(r^2 + \lambda^2 z^2). \tag{2}$$

The anisotropy of the trap is governed by the ratio λ between the axial and radial trapping strengths, so that when λ is larger than unity, the atomic cloud resembles a pancake and when $\lambda < 1$, it is cigar shaped. We shall see that the system behaves very differently in these two limits. The inter-particle interactions are parametrized by an s-wave scattering length a, so that $U_0 = 4\pi\hbar^2 a/m$. Combining these parameters into dimensionless quantities, we see that the physics of the system is entirely determined by λ and the effective coupling strength $C = 4\pi Na/a_{\rm osc}$, where $a_{\rm osc}$ is the harmonic oscillator length, $a_{\rm osc}^2 = \hbar/(m\omega_\perp)$. Since the chemical potential μ is a monotonically increasing function of C, it is possible to switch to the pair of parameters (λ, μ) instead of (λ, C). This more physical parameter choice is used in most of this paper. We now switch to dimensionless units in which energy is measured in units of $\hbar\omega_\perp$, frequency in units of $\omega_\perp$ and length in units of $a_{\rm osc}$. The Gross-Pitaevskii equation becomes

$$\left[-\frac{1}{2}\nabla^2 + \frac{1}{2}(r^2 + \lambda^2 z^2) + C|\Psi|^2\right]\Psi = \mu\Psi. \tag{3}$$

We shall, however, find it physically motivated to reinsert units when discussing physical scales throughout the paper.

For a given stationary solution Ψ_0 of the Gross-Pitaevskii equation with eigenvalue μ, the small-amplitude excitations of the condensate are described by the eigenvectors and eigenvalues of the Bogoliubov equations,

$$B\varphi_n(\mathbf{r}) = \omega_n \varphi_n(\mathbf{r}), \tag{4}$$

where $\varphi_n(\mathbf{r}) = (u_n(\mathbf{r}), v_n^*(\mathbf{r}))^T$, and the linear operator B is defined by

$$B = \begin{pmatrix} -\frac{1}{2}\nabla^2 + V(\mathbf{r}) - \mu + 2C|\Psi|^2 & C\Psi^2 \\ -C(\Psi^*)^2 & -\left(-\frac{1}{2}\nabla^2 + V(\mathbf{r}) - \mu + 2C|\Psi|^2\right) \end{pmatrix}. \tag{5}$$

B is non-Hermitian and may have complex eigenvalues. If this is the case, the system is dynamically unstable and the corresponding modes will grow exponentially. For the problem at hand, where Ψ is assumed to contain a doubly quantized vortex at the origin, it is known in the two-dimensional limit that there exist intervals of the coupling constant C where exactly one pair of eigenvalues is complex; in these intervals the doubly quantized vortex is unstable towards splitting, and between them it is dynamically stable. On the other hand, in the strongly cigar shaped limit, the experiment of Ref. [3] saw instability for all coupling strengths. In this paper, we shall see how these two situations emerge as the extreme limits of the general three-dimensional problem.

The "inner product" of two Bogoliubov eigenvectors φ_n is defined with the help of the Pauli matrix $\sigma_z = \mathrm{diag}(1, -1)$ as

$$\langle \varphi_m | \sigma_z | \varphi_n \rangle = \int d^3r \left(u_m(\mathbf{r})^* u_n(\mathbf{r}) - v_m(\mathbf{r})^* v_n(\mathbf{r}) \right). \tag{6}$$

The "norm" of a Bogoliubov eigenvector φ_n with respect to this "inner product", $\langle \varphi_n | \sigma_z | \varphi_n \rangle$, can be either positive, negative or zero, since it obeys the relation

$$(\omega_n - \omega_n^*) \langle \varphi_n | \sigma_z | \varphi_n \rangle = 0. \tag{7}$$

If ω_n is complex, the norm must be zero. In the case of real ω_n it may be either positive or negative and we shall fix normalization such that its absolute value is unity for all modes with real eigenvalue. Note that for every solution $\varphi_n = (u_n, v_n^*)^T$ of the Bogoliubov equation with eigenenergy ω_n, there exists a solution $\tilde{\varphi}_n = (v_n^*, u_n)^T$ with eigenvalue $-\omega_n^*$. If Ψ is the ground state of the Gross-Pitaevskii equation in the absence of rotation, the norm of each mode φ_n is equal to the sign of the corresponding ω_n, but that result does not hold for a general Ψ. The existence of modes with positive norm and negative energy (and necessarily also vice versa) signifies that there exist states with lower energy than Ψ (see Appendix A and [11, 12]).

If the problem is cylindrically symmetric and the condensate has an angular momentum M per particle, the excitations can be labeled by an angular momentum quantum number m relative to that of the condensate, such that

$$
\begin{aligned}
u(r,\theta,z) &= e^{i(M+m)\theta}u(r,z), \\
v(r,\theta,z) &= e^{i(M-m)\theta}v(r,z).
\end{aligned} \tag{8}
$$

The Bogoliubov eigenvalue problem thus splits up into a block diagonal matrix where the blocks corresponding to different m are decoupled. This allows us to treat each m value separately; the m'th sector of the Bogoliubov matrix takes on the form

$$
B = \begin{bmatrix} D_1 + V_d(r,z) & V_c(r,z) \\ -V_c(r,z) & -\left(D_2 + V_d(r,z)\right) \end{bmatrix}, \tag{9}
$$

where

$$
\begin{aligned}
D_1 &= \frac{1}{2}\left(-\frac{\partial^2}{\partial r^2} - \frac{1}{r}\frac{\partial}{\partial r} + \frac{(M+m)^2}{r^2} + \frac{\partial^2}{\partial^2 z}\right), \\
D_2 &= \frac{1}{2}\left(-\frac{\partial^2}{\partial r^2} - \frac{1}{r}\frac{\partial}{\partial r} + \frac{(M-m)^2}{r^2} + \frac{\partial^2}{\partial^2 z}\right),
\end{aligned} \tag{10}
$$

and the diagonal and off-diagonal potentials are defined as

$$
\begin{aligned}
V_d(r,z) &= V(r,z) - \mu + 2C|\Psi(r,z)|^2, \\
V_c(r,z) &= C|\Psi(r,z)|^2.
\end{aligned} \tag{11}
$$

For the problem at hand, the $m = 2$ sector will turn out to be especially interesting, as we shall see in the following sections.

In Appendix A it is shown how the present problem connects with Hamiltonian stability theory. It is seen that when two Bogoliubov eigenvalues become degenerate as a control parameter is changed, they will turn complex if they have opposite norm and the system thus turns dynamically unstable in the absence of further symmetries; in the case of equal norms there appears instead an avoided crossing. In this section we shall arrive at the same result in somewhat lesser generality. Consider two Bogoliubov amplitudes φ_j, with $j = 1, 2$, that solve the Bogoliubov equations for some pair of parameter values λ, C. We assume that the corresponding eigenvalues ω_j are real. Now slightly increase C to a value $C' = C + \delta C$, so that the ground-state solution Ψ becomes $\Psi' = \Psi + \delta\Psi$, and the Bogoliubov matrix is correspondingly written $B' = B + \delta B$. Now consider the restricted Bogoliubov problem in the truncated basis formed by φ_1, φ_2. (The validity of this approach shall shortly be determined.) Writing the ansatz as $\varphi = a_1\varphi_1 + a_2\varphi_2$, there results the eigenvalue problem for the vector $\boldsymbol{a} = (a_1, a_2)^T$,

$$\begin{pmatrix} \langle\varphi_1|\sigma_3|\varphi_1\rangle & 0 \\ 0 & \langle\varphi_2|\sigma_3|\varphi_2\rangle \end{pmatrix} \begin{pmatrix} \omega_1 + \delta B_{11} & \delta B_{12} \\ \delta {B_{12}}^* & \omega_2 + \delta B_{22} \end{pmatrix} \boldsymbol{a} = \omega \boldsymbol{a}, \tag{12}$$

where $\delta B_{ij} = \langle\varphi_i|\delta B|\varphi_j\rangle$. The eigenvalues are

$$\begin{aligned} \omega_\pm &= \frac{\omega_1 + \delta B_{11} + \omega_2 + \delta B_{22}}{2} \\ &\pm \left[\left(\frac{\omega_1 - \omega_2 + \delta B_{11} - \delta B_{22}}{2} \right)^2 + \langle\varphi_1|\sigma_3|\varphi_1\rangle\langle\varphi_2|\sigma_3|\varphi_2\rangle|\delta B_{12}|^2 \right]^{1/2} . \end{aligned} \tag{13}$$

It is seen that the eigenvalues can be substantially altered only if the eigenenergies ω_i are of the same order of magnitude as the perturbations δB_{ij}; thus one only has to care about the coupling between nearby energy levels, so the truncation of the basis to two states is justified. When the two modes have equal norm, they experience an avoided crossing. Conversely, a condition for the eigenvalues to be complex is that the two modes have different norm, $\langle\varphi_1|\sigma_3|\varphi_1\rangle\langle\varphi_2|\sigma_3|\varphi_2\rangle = -1$. Thus it can be concluded that a dynamic instability is formed by the mixing of a Bogoliubov mode of positive norm with one of negative norm (or states with opposite Krein signature in the language of App. A); when their energies coincide they go over to a pair of zero-norm modes with eigenenergies that are complex conjugates of each other. We will see plenty of examples of this phenomenon in the following.

For the numerical solution of the Bogoliubov equations, we employ the following method. At each point in the (λ, μ) phase space, the stationary solution of the Gross-Pitaevskii equation (1) is sought under the condition that it contains a doubly quantized vortex at the origin, so that the wave function is assumed to be of the form

$$\Psi(r, \theta, z) = e^{2i\theta}\Psi(r, z). \tag{14}$$

After that, the Bogoliubov problem is a matter of finding the eigenvalues to a $2n \times 2n$ matrix, where n is the size of the numerical grid. The spatial coordinates are discretized in a discrete-variable representation (DVR) [8, 9] using a Laguerre mesh for the radial direction and a Hermite mesh for the axial direction. For the solution of the two-dimensional problem reported in Secs. III and VII, the z dependence drops out and a one-dimensional Laguerre mesh is employed.

III. TWO-DIMENSIONAL CASE REVISITED

We first consider the case of a two-dimensional condensate, which can be realized in a strongly pancake-shaped trap, i. e. in the limit of large λ. In this limit, the condensate is in the harmonic-oscillator ground state in the z direction; integrating out the z-dependence, one obtains the effective coupling constant $\tilde{C} = C\lambda^{1/2}/\sqrt{2\pi}$. However, we find it physically more motivated to state our results in terms of the chemical potential μ, which is a monotone function of $\tilde{C}$ (although a closed expression for the dependence is known only in the limits of very small and very large $\tilde{C}$).

In the two-dimensional case it is known that the doubly quantized vortex is dynamically unstable only in certain intervals of the coupling strength [4]. The first instability sets in at zero coupling, as can be seen by considering the restricted eigenvalue problem, Eq. (12), for the lowest-lying eigenstates of the noninteracting problem, such that $\varphi_1 = (\phi_{400}, 0)^T$ and $\varphi_2 = (0, \phi_{000})^T$, where $\phi_{l,n_r,n_z}(r, \theta, z)$ are the harmonic-oscillator eigenstates in cylindrical coordinates. These two eigenstates are degenerate with Bogoliubov eigenvalue $\omega = 2$ in the noninteracting limit. For any finite coupling strength $\tilde{C}$, the Bogoliubov eigenvalues calculated from Eq. (12) turn complex. In order to determine the point where the system turns dynamically stable again, one has to consider the contributions from states with higher n_r [5].

Figure 1 shows the numerically computed real parts of the Bogoliubov eigenenergies as functions of the chemical potential μ in two dimensions. According to Eq. (13), the merging of two lines into one signifies the onset of instability, as two real energies become a complex conjugate pair. It is seen how the successive instability windows arise from the coupling of one mode, whose energy increases monotonously, with successive higher radially excited modes. This mode has no radial nodes and has negative norm in the intervals

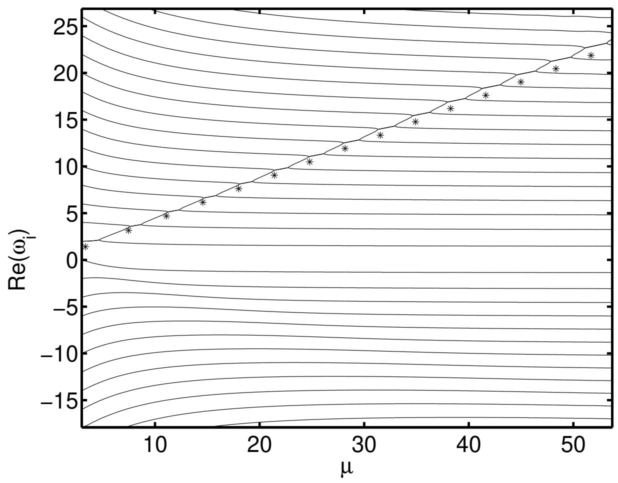

FIG. 1: Energy levels in two dimensions for $m = 2$. The $*$ represent the analytical appoximation to the crossing of the core mode with the trap modes shown in Eq. (17).

where its energy is purely real; we refer to it as the core mode since it is confined to the core of the doubly quantized vortex and effects in a splitting of the vortex into two. Its physical significance is that the doubly quantized vortex is *energetically* unstable to splitting into two, which furthermore causes dynamical unstability in certain windows of parameter space. As the coupling increases, the energy of the vortex is negligible compared with the energy contributions from the interaction and trapping potential. Therefore all the Bogoliubov energy levels approach the excitation energies for a two-dimensional condensate in the Thomas-Fermi limit [13, 14] , except for the core mode whose (real part of its) energy increases with increasing μ. In fact, the dependence of the core mode energy on the chemical potential is approximately linear. This can be intuitively understood as follows. If the core mode is populated, the doubly quantized vortex is split into two. The energy of the core mode corresponds to the frequency of the precession of the two vortices (since it determines the rate of change of the relative phase of the condensate wave function and the Bogoliubov mode). At the same time, we know that two vortices of equal vorticity will precess around each other with a velocity proportional to the inverse of their separation, and the angular frequency of this precession is thus $\omega_{\text{prec}} = \hbar/(mr_{12}^2)$. Inserting for r_{12} the healing length ξ, which is the size of a vortex core, one obtains indeed $\hbar\omega_{\text{prec}} \propto \mu$.

A more quantitative estimate of the core mode energy can be obtained in the limit of a large condensate. Consider the Bogoliubov equation (4) with Eq. (9) inserted for the matrix operator B, and neglect the z depencence. We do the analysis for a general set of quantum numbers M, m before specializing to the currently relevant case $M = m = 2$. The diagonal and off-diagonal effective potentials $V_d(r)$ and $V_c(r)$ defined in Eq. (9) are sketched in Fig. 2 using the Thomas-Fermi approximation [1] for the condensate wavefunction. Since the norm of the core mode φ is negative, it is dominated by its lower index v. If its eigenvalue ω is positive, as we expect it to be, the amplitude v is concentrated to the vortex core, i. e. the innermost potential well of the potential V_d, while the upper component u experiences an additional centrifugal potential which makes its overlap with v and the off-diagonal potential V_c exceedingly small. This justifies the term "core mode" for this mode, and we therefore

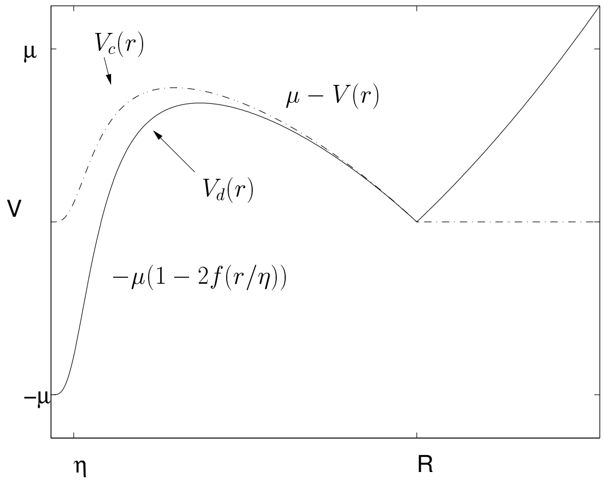

FIG. 2: The effective diagonal (full line) and off-diagonal (dashed) potentials experienced by the Bogoliubov modes, defined in Eq. (9). Centrifugal potentials are not included in the definition.

denote the amplitude by v_{core} and the corresponding energy by ω_{core}. Moreover, in the limit of a large condensate, the extent of the function $v_{\text{core}}(r)$ is of order ξ and the trapping potential contributes little to its eigenenergy. Hence the Bogoliubov equation for the core mode can be well approximated by the diagonal term,

$$\left[\frac{\hbar^2}{2m}\left(-\frac{\partial^2}{\partial r^2} - \frac{1}{r}\frac{\partial}{\partial r} + \frac{(M-m)^2}{r^2}\right) - \mu + 2U_0|\Psi(r)|^2\right] v_{\text{core}}(r) = -\omega_{\text{core}} v_{\text{core}}(r). \tag{15}$$

The condensate wave function Ψ can be written as the product of the square root of the density away from the core, n_0, and a core function $f(r)$ describing how Ψ goes to zero due to the centrifugal force: $\Psi(r) = \sqrt{n_0} f(r)$. The density n_0 is unaffected by the trapping potential at distances r comparable to ξ, and is assumed constant; it is related to the chemical potential by $\mu = U_0 n_0$. Rescaling the length, $r = \xi x$, results in the equation

$$\left[\frac{1}{2}\left(-\frac{\partial^2}{\partial x^2} - \frac{1}{x}\frac{\partial}{\partial x} + \frac{(M-m)^2}{x^2}\right) - \frac{1}{2} + f(x)^2\right] v_{\rm core}(x) = -\frac{\omega_{\rm core}}{2\mu} v_{\rm core}(x). \qquad (16)$$

Already from here one can see that since all parameters are scaled away from the left-hand side, $\omega_{\rm core}/\mu$ must be a constant, i. e. the core mode energy is proportional to the chemical potential. A variational quantitative estimate can be obtained as follows. Assuming a general condensate with angular momentum M and modeling $f(x)$ as a linearly increasing function cut off at the position $x = b$, we obtain by variational means $b = M\sqrt{6}$ [10]. With this assumption for the function f, the solutions $v_{\rm core}$ to Eq. (16) are harmonic-oscillator eigenfunctions and the eigenenergies come out as

$$\frac{\omega_{\rm core}}{\mu} = -(2n_r + (M-m) + 1)\frac{2}{M\sqrt{3}} + 1. \qquad (17)$$

Since the analysis is only assumed to hold for positive-energy states, we put $n_r = 0$ for $M = 2$. The estimate is in excellent agreement with numerical solutions of Eq. (16) with the numerically calculated condensate wavefunction inserted. This energy is indeed positive for $M \geq 2$ and $m \geq 0$, i. e. of opposite sign compared to the norm. (Recall that we could equally well have considered the corresponding Bogoliubov mode with $m \to -m$ and the upper component u confined to the core; it has positive norm and negative energy.)

The above estimate is readily checked against the numerical result for a two-dimensional trapped condensate in the strong-coupling regime. We read off the numerically calculated core mode energy at the arbitrarily chosen point $\mu = 40\hbar\omega_\perp$. For the $m = 2$ core mode in a condensate with $M = 2$, we obtain the variational estimate $\omega_{\rm core} = 0.423\mu$, while the numerical result is $\omega_{\rm core} = 0.438\mu$. For $m = 3$ and $M = 3$, we obtain variationally $\omega_{\rm core} = 0.615\mu$ and numerically $\omega_{\rm core} = 0.665\mu$, and for the $m = 4$ core mode in a $M = 4$ condensate the variational result is $\omega_{\rm core} = 0.711\mu$ and the numerical result is $\omega_{\rm core} = 0.781\mu$.

The positions of the successive instability windows can now be estimated by calculating the crossing of the core mode with quadrupole modes with increasing radial quantum numbers n_r. The energies of the latter will in the limit of strong coupling not depend on the multiply quantized vortex in the center of the condensate, so we can use the values calculated for a nonrotating two-dimensional condensate [13, 14]

$$\omega_{n_r,m} = \hbar\omega_\perp\sqrt{2n_r^2 + 2n_r m + 2n_r + m}. \qquad (18)$$

The variational estimates for the crossings, i. e. the points μ where $\omega_{\rm core} = \omega_{n_r,m}$ for $m = 2$ and some n_r, are indicated in Fig. 1. It is possible to proceed and calculate the overlap between the core and quadrupole modes, which yields the widths of the unstable windows and the imaginary parts of the eigenfrequencies. However, this is impossible in practice, since the integrand in the relevant integral initially goes as the sixth power of the coordinate, and the result will be extremely sensitively dependent on the width of the core mode, which is a variational parameter. We will therefore not pursue this analysis.

IV. INSTABILITY REGIONS FOR A THREE-DIMENSIONAL CONDENSATE

Figure 3 contains the main result of this study. Displayed is the largest imaginary part

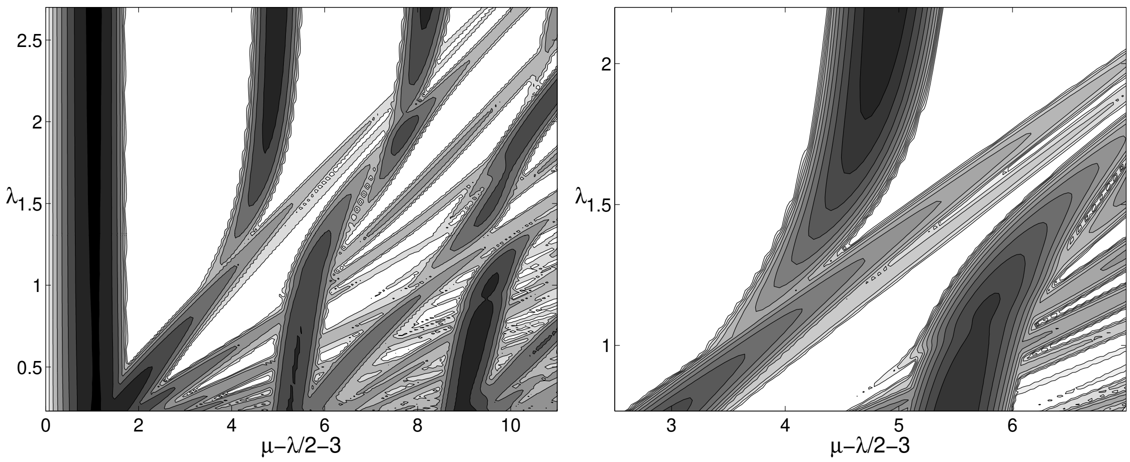

FIG. 3: Unstable regions for a doubly quantized vortex in the parameter space of trap anisotropy λ and chemical potential μ; the latter is downshifted by its value at zero coupling, $3 + \lambda/2$. The shading indicates the highest of the imaginary parts of the Bogoliubov eigenvalues. White is zero which means that the condensate is stable.

of the Bogoliubov eigenenergies as a function of parameters μ, λ. All the unstable modes are in the $m = 2$ sector, there are no unstable modes with quantum number $m \neq 2$. An instability with $m = 2$ corresponds to a splitting of the doubly quantized vortex line into two single vortex lines, as can be seen by considering the density profile of a superposition of $m = 2$, $m = 0$ and $m = 4$ radial eigenfunctions. Note that we have chosen the coordinate along the abscissa to be the chemical potential μ, downshifted by its value at zero coupling, $3 + \lambda/2$. With this coordinate choice, the instability regions in the large-λ limit appear as vertical stripes, as we shortly discuss. The instability regions bounded by straight diagonal lines are instabilities between negative energy states $n_r = 0, n_z = n_n$ and positive energy states $n_r = 0, n_z = n_p$ with $n_n - n_p$ even. They correspond to instabilities with axial nodes. In the next section we shall study these instabilities in greater detail.

The alternating stability and instability regions known from previous two-dimensional studies [4–6] and discussed in Sec. III are clearly seen in the pancake shaped, large λ limit as vertical stripes. We refer to these as 2D instabilities, since they arise from dynamics in the plane. When λ approaches unity from above, one sees how the 2D instability regions become distorted. In fact, the distortion of the second vertical stripe can be explained as an avoided crossing phenomenon. As discussed in Sec. III, it is the crossing of the $n_r = 1$, $n_z = 0$ mode with the $n_r = 0$, $n_z = 0$ core mode in the oblate limit that gives rise to the second vertical stripe. On the other hand, in the cigar shaped limit the instability of the $n_r = 0$, $n_z = 2$ mode with the $n_r = 0$, $n_z = 0$ core mode appears as a diagonal band in the lower part of Fig. 3, as we discuss in Sec. V. The two modes ($n_r = 1$,$n_z = 0$) and ($n_r = 0$, $n_z = 2$) have the same symmetry and positive norm, and will mix when their energy is similar, giving rise to an avoided crossing around $\lambda = 1$. This avoided crossing of the real energy levels is shown in Fig. 4 for $\lambda = 1.2$. The two modes in question start off at $\mu - \lambda/2 - 3 = 0$ as harmonic-oscillator eigenstates with energies $\omega_{n_r=1,n_z=0} = 4$ and $\omega_{n_r=0,n_z=2} = 2+2\lambda = 4.4$, respectively. The lines can be seen to undergo an avoided crossing around $\mu = 0.5$; the exact position of this crossing depends on λ. Furthermore, both of these eigenmodes become unstable when they cross with the core mode, the negative-norm eigenmode $n_r = 0, n_z = 0$. The result is an avoided crossing of the instability regions. In the right panel of Fig. 3 the instabiliy region in the high λ region corresponds to $n_r = 1, n_z = 0$; this goes continously over to $n_r = 0, n_z = 2$ in the lower left corner, while we find the $n_r = 1, n_z = 0$ state again as the strong instability in the region between $5 \lesssim \mu - \lambda/2 - 3 \lesssim 6$ in the lower part of the figure. Of course, one has to keep in mind that the quantum numbers n_r, n_z only make sense in the weak coupling limit. Their meaning is lost in the strong-coupling limit, where the r and z dependence is no longer separable, but it remains a convenient way to label the states.

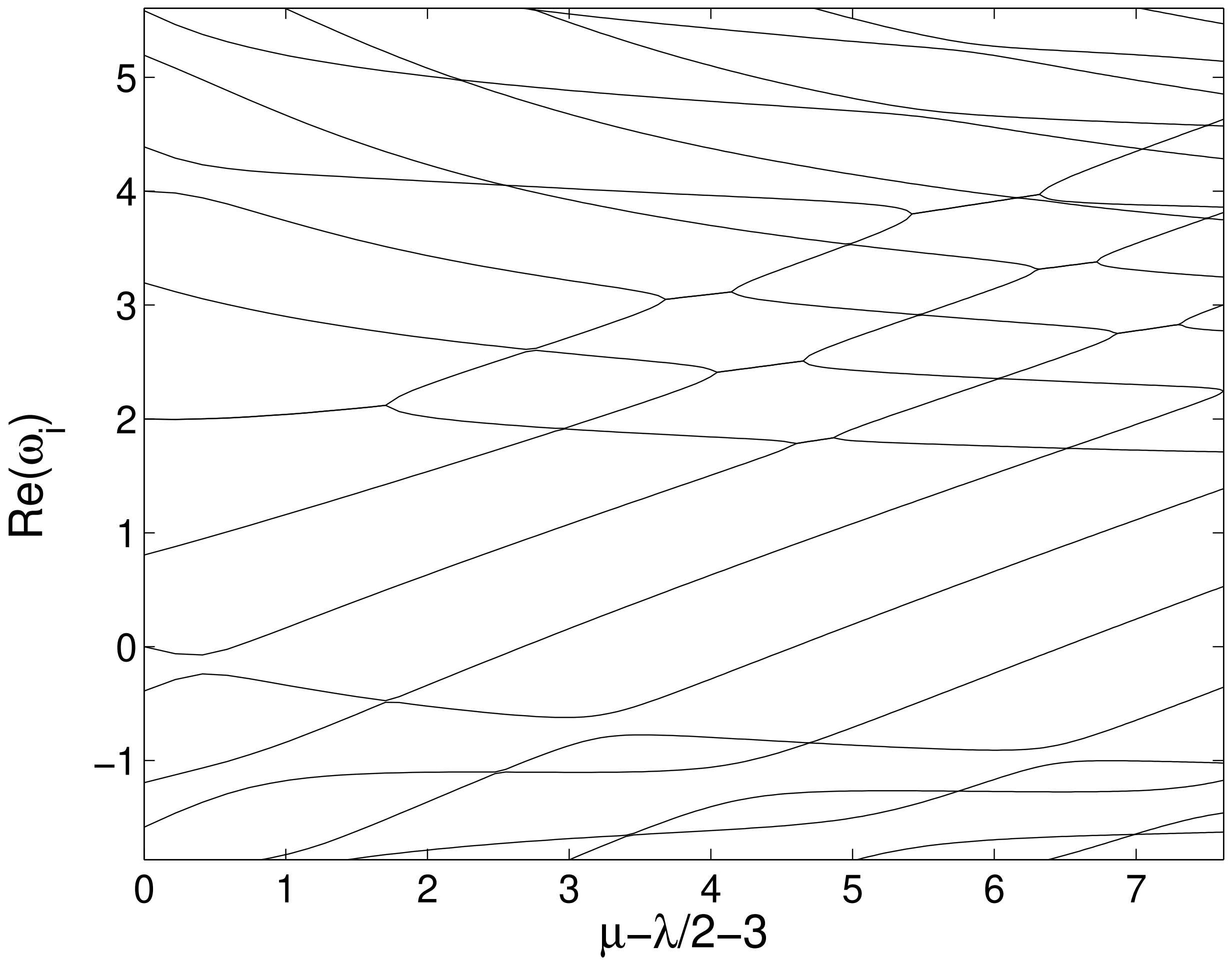

FIG. 4: Real parts of the Bogoliubov eigenenergies as functions of the chemical potential μ for the trap anisotropy $\lambda = 1.2$, i. e., an almost isotropic trapping potential.

V. INSTABILITY IN THE CIGAR SHAPED LIMIT

When $\lambda \ll 1$, the condensate obtains an elongated, cigar-like shape. In this limit the lowest-energy excitations are in the z direction, since their energy separation is $\lambda\hbar\omega_\perp$ while the radial excitation energy is equal to $\hbar\omega_\perp$. The problem is thus one-dimensional as long as radial excitations can be neglected. The instability regions carrying different quantum numbers n_z are seen to spread out like a fan in the lower part of Fig. 3. The analysis in the previous paragraph still holds for the $m = 2, n_r = n_z = 0$ instability, which sets in at zero coupling also in the cigar shaped limit. Because of parity, this mode does not mix with the modes that have odd axial quantum numbers n_z and we now deal with those separately. Consider again the Bogoliubov equation restricted to the space spanned by two nearby modes, Eq. (12). Assuming that perturbation theory holds so that harmonic-oscillator eigenfunctions can be used, we insert into Eq. (12) the trial Bogoliubov amplitudes $\varphi_1 = (\phi_{401}, 0)^T$ and $\varphi_1 = (0, \phi_{001})^T$, where we remind the reader that the harmonic-oscillator eigenfunctions ϕ_{l,n_r,n_z} are indexed with the azimuthal, radial, and axial quantum numbers in turn. The calculation shows that the mode is unstable when

$$\frac{512\pi^{3/2}}{17\sqrt{2}+8\sqrt{3}} < \frac{\tilde{C}}{\lambda} < \frac{512\pi^{3/2}}{17\sqrt{2}-8\sqrt{3}}. \tag{19}$$

We rephrase this in terms of the chemical potential, which in the weak-coupling limit varies as $\mu = 3 + \lambda/2 + 3\tilde{C}/[3(2\pi)^{3/2}]$. There results

$$\frac{12}{17+4\sqrt{6}} < \frac{\mu - \lambda/2 - 3}{\lambda} < \frac{12}{17-4\sqrt{6}}. \tag{20}$$

Thus, the fan-like structure in the lower part of Fig. 3 should be bounded from the left by the ray $\lambda \approx 0.6002(\mu - \lambda/2 - 3)$. Although the boundary of this instability region appears fairly straight, its slope is about half the value predicted by this weak-coupling analysis. This is because the instability sets in at a coupling strength where many more harmonic-oscillator eigenfunctions are already mixed into the relevant Bogoliubov modes. Going to the limit of small λ and small μ does not help, since the above analysis indicates that the instability sets in only when the interaction energy, which is proportional to the shift in chemical potential $\mu - \lambda/2 - 3$, is of the order of the the harmonic-oscillator level spacing $\lambda\hbar\omega_\perp$.

Figure 5 shows the real parts of the Bogoliubov eigenenergies as functions of the coupling for the fixed anisotropy $\lambda = 0.2$. It is clearly seen that the radially excited states, in the upper part of the figure, are well separated from the lowest axially excited states and thus they do not affect the dynamics in the weak-coupling limit. Again, the simplest way to determine the quantum numbers of a particular mode is to inspect its energy in the noninteracting limit. The two modes that in the noninteracting limit have energies $\omega = (2\pm\lambda)\hbar\omega_\perp = (2\pm0.2)\hbar\omega_\perp$ are the ones with quantum number $n_z = 1$. The initial linear behavior of the energies can be obtained from the harmonic-oscillator eigenfunction analysis in the previous paragraph, but the curvature of the lines becomes important, and as a result the levels merge at a higher chemical potential than predicted by the weak-coupling analysis.

As discussed above, the merging of the two lines into one signifies the onset of instability, where according to Eq. (13) the two real energies become a complex conjugate pair. At a somewhat larger μ the modes with $n_z = 2$ merge and become complex. The levels split

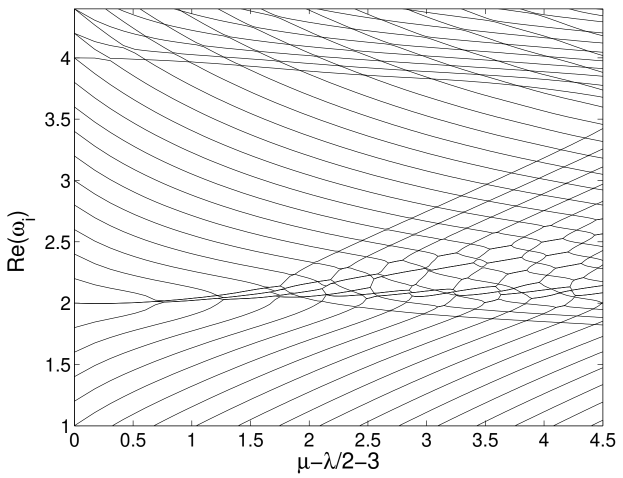

FIG. 5: Real part of the Bogoliubov energy spectrum for the case $\lambda = 0.2$, i. e., in the limit of a cigar shaped condensate.

apart and become purely real again for a larger value of μ. As long as the system is approximately one-dimensional in the sense that radial excitations are well separated from the axial ones, the curves presented in Fig. 5 are universal and are only dilated by a factor λ as the anisotropy is changed. As a result, the instability boundaries appear as straight lines that give rise to the fan-shaped structure in Fig. 3.

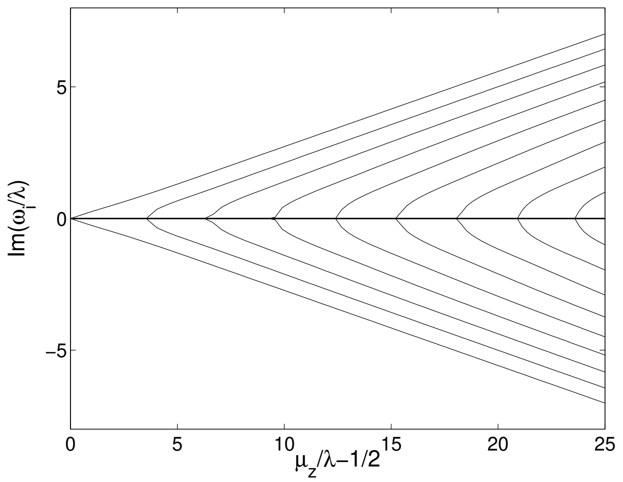

FIG. 6: Imaginary parts of the Bogoliubov eigenvalues, $Im(\omega_i)$, in the limit of weak interaction and strongly cigar-shaped geometry, calculated using the one-dimensional model defined in Eq. (21).

If we go to the extreme cigar limit, we can completely ignore the excitations in the radial direction. The Bogoliubov equation will in this case be an eigenvalue problem of two coupled one-dimensional differential equations. For convenience we define $\mu_z = \mu - (3 + \lambda/2)$, where the subscript implies that the change in chemical potential as the coupling is increased arises here from the dynamics in the z direction. Inserting the lowest radial harmonic-oscillator eigenfunctions for Ψ, u and v in the Bogoliubov matrix operator, Eq. (9), integrating out the radial direction and redefining units by putting $\tilde{z} = (\lambda z)/\sqrt{2\mu_z}$ and the axial condensate function $\Psi(z) = \mu_z \tilde{\Psi}(z)/C$ we obtain

$$\begin{bmatrix} -\frac{1}{(\frac{\mu_z}{\lambda})^2}\frac{\partial^2}{\partial \tilde{z}} + 2\frac{5}{8}|\tilde{\Psi}|^2 - 1 & \frac{1}{\sqrt{6}}|\tilde{\Psi}|^2 \\ -\frac{1}{\sqrt{6}}|\tilde{\Psi}|^2 & -\left(-\frac{1}{(\frac{\mu_z}{\lambda})^2}\frac{\partial^2}{\partial \tilde{z}} + 2\frac{2}{3}|\tilde{\Psi}|^2 - 1\right) \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} = \frac{\omega_i}{\mu_z} \begin{bmatrix} u \\ v \end{bmatrix}. \tag{21}$$

If we furthermore assume that the Thomas-Fermi (TF) approximation [1] for the condensate wavefunction is valid in the z direction, the peak value of $\tilde{\Psi}$ is just equal to 1, and the only remaining parameter in the equation is μ_z/λ. Thus the points at which the different axial modes becomes complex are given by μ_z/λ = const, i.e, straight lines in figure 6. Furthermore, in the limit $\mu_z/\lambda \to \infty$ we can neglect the derivative of the function at the center of the trap and the eigenvalues ω_i/μ_z have to approach the eigenvalues of the matrix

$$A = \begin{bmatrix} \frac{1}{4} & \frac{1}{\sqrt{6}} \\ -\frac{1}{\sqrt{6}} & -\frac{1}{3} \end{bmatrix}. \tag{22}$$

The result is $\omega_i = \mu_z(-1/24 \pm i\sqrt{47}/24) - O(\lambda)$. In the actual two-dimensional situation we have seen that the imaginary parts of the frequencies rise to a maximum value and then decrease to zero; this behavior is not predicted by the 1D model and is thus a two-dimensional effect. In order to estimate the maximum values of the imaginary parts of the frequencies, we observe that the radial dynamics is expected to begin to matter when μ exceeds unity, so putting $\mu_z = 1$ gives an estimate $\mathrm{Im}(\omega_i) \sim 0.3$. The actual value from the three-dimensional calculation turns out to be 0.14 for the maximum of the first imaginary frequency, with a slight dependence on λ. We conclude from the one-dimensional calculation that the periodic regions of stability and the maximum of the imaginary part of the eigenvalue is an effect arising from the dynamics in the radial direction.

It is again instructive to visualize the instability by considering the shape of the wave function $\psi(r, \theta, z)$ with a small admixture of the Bogoliubov amplitudes u and v. One sees that the $m = 2, n_z = 0$ modes simply correspond to a straight splitting of the doubly quantized vortex into two. The $m = 2, n_z = 1$ mode corresponds to two vortices that split at the edges of the condensate, at large $|z|$, but are joined at $z = 0$, thus forming an X-shaped structure. In experiments one will generally be in a regime where more than one mode is unstable. This will result in a intertwining of two vortices. This was studied numerically in Refs. [6, 7]. The splitting was found to nucleate in certain intervals of z, corresponding in the present picture to a high quantum number n_z, as is expected for strong coupling. The ensuing intertwining of the two vortices originates from higher-order effects such as coupling between different modes. It was also proposed in Refs. [6, 7] that the criterion for local splitting can be found from a local-density approximation of sorts, by treating the elongated condensate as a stack of two-dimensional slices. If the local density integrated over the xy plane matches the instability criterion for the two-dimensional system, an instability will be nucleated at that point. This kind of analysis presumably holds in the limit of a large condensate, where local-density approximations are expected to hold, but we shall not pursue that analysis.

VI. COMPARISON WITH EXPERIMENT

The experiment by Shin et. al. [3] was done with aspect ratios λ ranging from 1/100 to 1/20. This is clearly in the cigar-shaped domain. In this region the unstable modes are quadrupole modes with axial nodes, as we have seen in the preceding section.

Figure 7 shows the value of the maximal complex eigenvalue (MCE) for $\lambda = 0.2$, as a function of the effective two-dimensional coupling strength an_z, which is the parameter that was used in Ref. [3]. Because of numerical limitations, we have used a larger value of λ than in the experiment, but as we have seen, the most important features, such as the position of the 2D instabilities, do not change when λ is decreased. In the region between the two 2D instabilities, states corresponding to successively higher numbers of axial nodes becomes the most unstable mode. The instability gets weaker with higher density in the region $0 < an_z < 12$, which is precisely the parameter interval that was scanned in the experiment. Clearly, because of a coincidence the experiment was performed in the parameter regime lying exactly between the two first 2D instabilities. As we saw in Sec. V, finding the maximum of the complex part of the eigenvalues (MCE) is a purely computational task, since a good analytical approximation seems to be difficult to construct. Qualitatively we can understand that the MCE decreases with increasing coupling because the coupling element is smaller when the unstable modes have axial nodes. To compare

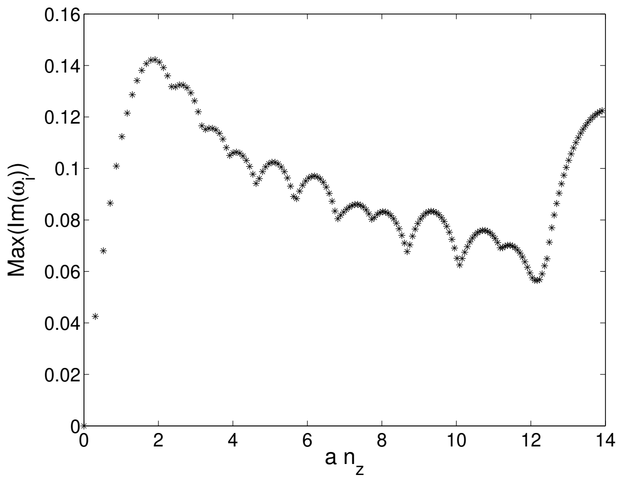

FIG. 7: The maximal complex eigenvalue for $\lambda = 0.2$. $an_z = a \int \Psi(r,0) 2\pi r dr$ where a is the scattering length.

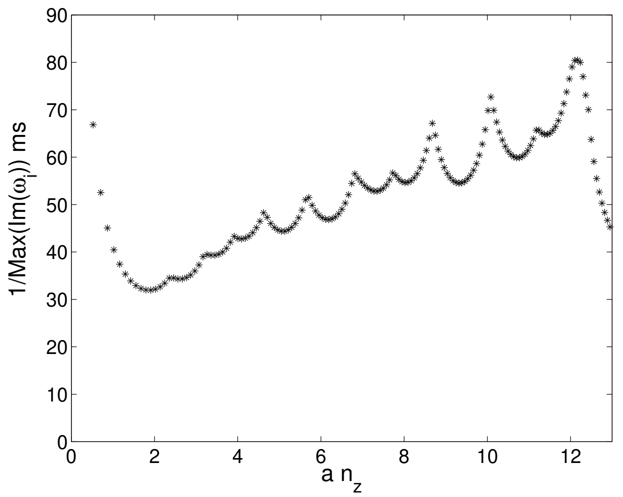

FIG. 8: The splitting time of a doubly quantized vortex for the experiment of Ref. [3]. We have used $\lambda = 0.2$ in the calculations.

with the experiment [3], we relate the lifetime of a doubly quantized vortex to the reciprocal of the MCE. The result is presented in figure 8 in the units used in the experiment. The two-dimensional coupling strength an_z is defined as $an_z = a \int \Psi(r,0) 2\pi r dr$, and has to be computed numerically for each data point. The numerical result has the correct qualitative behavior, and the quantitative scale is also similar to the experimental result. In Ref. [7], a real-time simulation of the splitting scenario was carried out, and the calculated splitting times are in qualitative agreement with the present results. We could not have expected a precise quantitative agreement, since the exact relationship between the complex eigenvalues and the splitting criteria used in [3] is unsure.

VII. STABILITY IN AN ANHARMONIC TRAP

In the previous sections we have studied a doubly quantized vortex in a harmonic trap. In this case the vortex becomes unstable already for an infinitesimal value of the coupling C. We have seen that this is due to the degeneracy of the eigenvalues in the harmonic trap. To understand the connection between the energy spectrum and the instability further, we now present the corresponding calculations for an anharmonic trap. We use the potential

$$V(r) = \frac{1}{2}r^2 + (\alpha r)^4 \,. \tag{23}$$

The regions of instability for this potential are shown in Fig. 10. The energies in the noninteracting limit are no longer degenerate as they were in the harmonic case: For a given anisotropy, the energy of the negative norm state is below the energy of the positive norm state for weak coupling. The nonlinear coupling therefore needs to attain a finite value in order for the two real eigenvalues to meet, so that the eigenvalues turn complex and the vortex becomes unstable. After this point the situation will be similar to the harmonic case, except that the mode frequencies are shifted, which causes a corrsponding shift in the positions of the unstable regions.

In the weak-coupling region, before the first complex eigenvalue appears, it is possible to find a rotating frame with rotation frequency Ω such that all the positive-norm and negative-norm states have positive and negative energy respectively, i.e., all modes have a positive Krein signature (see App. A). If this is the case for all sectors with different angular momentum quantum number m (which, in fact, it is for certain Ω and C values), then the the doubly quantized vortex is energetically stable in that rotating frame. This certainly implies that the vortex is stable (both linearly and nonlinearly), both to perturbations of the vortex state and also to perturbations of the Hamiltonian that are rotational symmetric.

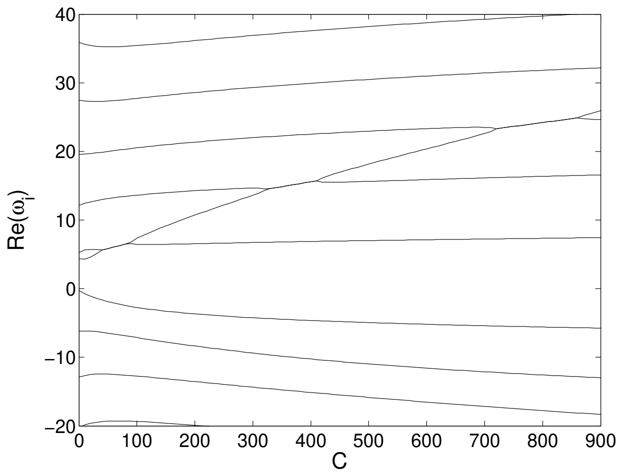

FIG. 9: Real part of the energy spectrum for the two-dimensional case in an anharmonic potential with anharmonicity parameter $\alpha = 0.92$.

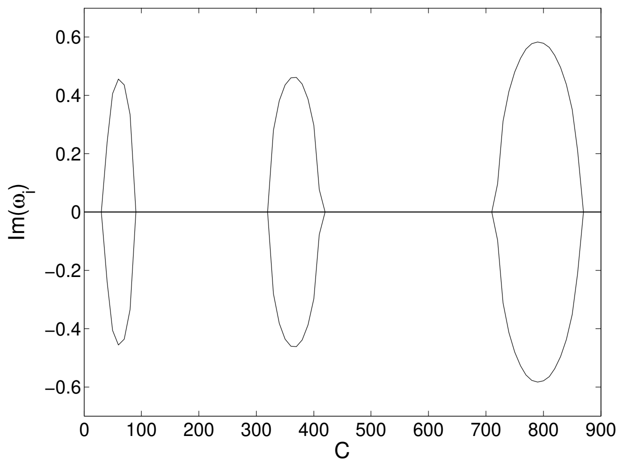

FIG. 10: Imaginary part of the energy spectrum for the two-dimensional case in an anharmonic potential with $\alpha = 0.92$.

VIII. CONCLUSIONS

We have in detail studied the excitation spectrum for a doubly quantized vortex in a trapped condensate. The instability regions were studied numerically for a wide range of trap shapes and interaction strength. For the previously studied two-dimensional case, which is expected to described pancake shaped condensates [4], we explained the instabilities in terms of level crossings between the core mode and the quadrupole modes of the condensates and found an analytical approximation for the position of the instability regions. A corresponding

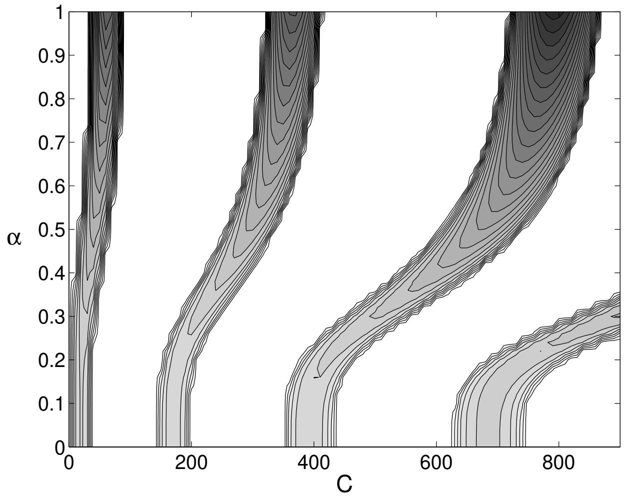

FIG. 11: Dynamic stability region for a doubly quantized vortex in an anharmonic trap, as a function of coupling strength C and anharmonicity α.

study of the anharmonic trap was carried out in order to point out the connections and differences between spectral and energetic stability.

We have systematically mapped out the regions of instability in a three-dimensional trap for a wide range of aspect ratio. In particular, we have given an explanation of the results of the experiment performed by Shin et. al. [3], which were performed in a cigar shaped geometry. In such a geometry, as the interaction strength becomes larger the modes responsible for the instability have successively more nodes in the axial direction. The coupling decreases with the number of nodes. This explains the increase of the splitting time with the interaction strength seen in the experiment. Our result also give the right magnitude of the splitting time.

APPENDIX A: RELATION BETWEEN HAMILTONIAN STABILITY THEORY AND BOGOLIUBOV THEORY

The Nonlinear Schrödinger equation (NLS) governing the order parameter Ψ for a condensed Bose gas can be written as

$$\begin{aligned} i\frac{\partial \Psi}{\partial t} &= \frac{\partial H_c}{\partial \Psi^*} \\ i\frac{\partial \Psi^*}{\partial t} &= -\frac{\partial H_c}{\partial \Psi} \end{aligned} \tag{A1}$$

where the Hamiltonian is $H_c = \Psi^* H_0 \Psi + 1/2C|\Psi|^4$. If one considers Ψ^*, Ψ as independent variables, this is already a system written in the standard form. However, one may also introduce real variables by defining $p = \mathrm{Im}(\Psi)$, $q = \mathrm{Re}(\Psi)$, and $H = H_c/2$. Then we can write the NLS in standard Hamiltonian form using real variables,

$$\begin{aligned} \frac{\partial p}{\partial t} &= -\frac{\partial H}{\partial q} \\ \frac{\partial q}{\partial t} &= \frac{\partial H}{\partial p}. \end{aligned} \tag{A2}$$

Before expanding about a stationary point it is convenient to introduce the symmetric matrices for the real and complex formulations of the problem, respectively,

$$L = \begin{bmatrix} \frac{\partial^2 H}{\partial p \partial p} & \frac{\partial^2 H}{\partial q \partial p} \\ \frac{\partial^2 H}{\partial \ q \partial p} & \frac{\partial^2 H}{\partial q \partial q} \end{bmatrix} \quad L_c = \begin{bmatrix} \frac{\partial^2 H_c}{\partial \Psi \partial \Psi^*} & \frac{\partial^2 H_c}{\partial \Psi^* \partial \Psi^*} \\ \frac{\partial^2 H_c}{\partial \Psi \partial \Psi} & \frac{\partial^2 H_c}{\partial \Psi \partial \Psi} \end{bmatrix} \tag{A3}$$

as well as the antisymmetric matrix, J, associated with the symplectic form, along with its counterpart in the complex formulation, the Pauli matrix associated with the non-definite norm defined for Bogoliubov states:

$$J = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \tag{A4}$$

Observe that $\sigma_z L_c$ is just the Bogoliubov matrix B defined in Eq. (5). If we expand the equation (A2) about a stationary solution we obtain the equation for the small deviation $d\Psi$,

$$i\frac{\partial}{\partial t} \begin{bmatrix} d\Psi \\ d\Psi^* \end{bmatrix} = \sigma_z L_c \begin{bmatrix} d\Psi \\ d\Psi^* \end{bmatrix}. \tag{A5}$$

If we search for eigenmodes of the right hand side we get the familiar Bogoliubov equation. In the real-variable formulation the expansion becomes

$$\frac{\partial}{\partial t} \begin{bmatrix} dp \\ dq \end{bmatrix} = JL \begin{bmatrix} dp \\ dq \end{bmatrix} \tag{A6}$$

The right hand side is the starting point for spectral analysis in the literature about Hamiltonian systems. The conversion between the two eigenvalue problems is found using the conversion between complex and real coordinates,

$$\begin{bmatrix} dp \\ dp^* \end{bmatrix} = \frac{1}{2} \begin{bmatrix} -i & i \\ 1 & 1 \end{bmatrix} \begin{bmatrix} d\Psi \\ d\Psi^* \end{bmatrix}, \quad \begin{bmatrix} d\Psi \\ d\Psi^* \end{bmatrix} = \begin{bmatrix} i & 1 \\ -i & 1 \end{bmatrix} \begin{bmatrix} dp \\ dq^* \end{bmatrix} \tag{A7}$$

This results in

$$\begin{bmatrix} -i & 1 \\ i & 1 \end{bmatrix} JL \begin{bmatrix} -i & i \\ 1 & 1 \end{bmatrix} = -i\sigma_z L_c \tag{A8}$$

The eigenvectors of JL give the eigenmodes of the NLS in the real-variable formulation and those of $\sigma_z L$ give the eigenmodes in the form we know from the Bogoliubov equation. Real eigenvalues of $\sigma_z L_c$ correspond to imaginary eigenvalues of JL. The Krein signature of an eigenvalue which plays an important role in the analysis of Hamiltonian systems, is defined as the sign of the energy change of the Hamilton restricted to the subspace spanned by the corresponding eigenvector. Suppose

$$JL\boldsymbol{\eta} = -i\lambda\boldsymbol{\eta} \quad \lambda \in R,\, \boldsymbol{\eta} = \boldsymbol{\eta}_r + i\boldsymbol{\eta}_i \tag{A9}$$

$$\sigma_z L_c \boldsymbol{\chi} = \lambda\boldsymbol{\chi} \quad \chi^T = [u, v]\,. \tag{A10}$$

Then the Krein signature is defined as

$$\mathrm{sign}(\langle\eta_r|L_c|\eta_r\rangle) = \mathrm{sign}\left(i\lambda\langle\eta|J|\eta\rangle\right) = \mathrm{sign}(\lambda\langle\eta_r|J|\eta_i\rangle) = \mathrm{sign}(\lambda\langle\chi|\sigma_z|\chi\rangle). \tag{A11}$$

Here we have used that

$$\begin{bmatrix} i & 1 \\ -i & 1 \end{bmatrix} J\frac{1}{2} \begin{bmatrix} -i & i \\ 1 & 1 \end{bmatrix} = -i\sigma_z. \tag{A12}$$

We see that the norm defined as $\langle\chi|\sigma_z|\chi\rangle$, which is usually introduced to ensure commutator rules while doing the Bogoliubov transformation [1], corresponds to the symplectic form in the Hamiltonian formulation. The Krein signature for a real eigenvalue is then the the sign of the product of the norm and the eigenvalue.

We now present some results from Hamiltonian dynamics in the language used in BEC research. These results are for the most part stated and proven for a finite system; we assume that the application of these to the infinite-dimensional NLS does not cause any problems.

First we state Krein's theorem:

Theorem 1 *Collisions of eigenvalues with equal Krein signature do not provoke instability. [15]*

This implies that if the eigenvalues of two Bogoliubov modes with equal Krein signature approach each other as the Hamiltonian is changed, they will stay real and can not become complex under a small perturbation. In other words, the eigenvalues can only become complex if a negative and positive norm eigenvalue collide.

The second theorem is called Moser's theorem when stated in the following form.

Theorem 2 *If the signatures of two colliding eigenvalues are mixed, then either the spectrum contains two complex conjugated eigenvalues or it can be made to have it with an arbitrarily small perturbation of the Hamiltonian.[16].*

This means that if two eigenvalues of opposite Krein signature collide they will either become complex or they can become complex under an arbitrarily small perturbation of the Hamiltonian. In our case two eigenvalues of opposite Krein signature can cross in two cases without causing instability. One case is if they have different parity in the z-direction. In this case it is the symmetry about the the z-axis which prevents the eigenvalues from becoming complex, i.e a arbitrarily small perturbation which destroys this symmetry will lead to complex eigenvalues. The other case is if the two eigenvalues correspond to different m values; again, the addition of a perturbation that breaks the rotational symmetry about the z axis will cause an instability in this case.

In general, spectral stability (i.e., all eigenvalues real) does not imply stability . In order for the system to be stable, the Krein signatures of all eigenvalues also need to be all positive (or negative). This will in our language mean that all eigenvalues with negative norm must have negative eigenvalues.

For a Hamiltonian which is invariant under a symmetry group G, we have to take care to define stability up to transformations in the symmetry group. The system in the current study obeys the symmetry group $U(1) \otimes U(1)$, where the first $U(1)$ group is associated with global phase rotations and the second is associated with the rotational symmetry of the Hamiltonian around the z-axis. If the rotational symmetry of the condensate Ψ were broken, this would imply that we had four zero eigenvalues, since the generators of the group will produce a zero eigenvalue when acting on the condensate. However, in our case, the condensate is cylindrically symmetric, which implies that the rotation of the doubly quantized vortex is equivalent to a phase change, and as a result we only have two zero eigenvalues. Stability in this context means stability up to a phase change. In general, for a system with a cylindrically asymmetric vortex lattice, it also means stability up to a rotation [17, 18].

If we find an external rotational frequency Ω such that the Bogoliubov equation in that rotating frame gives only positive Krein signatures, except for the zero eigenvalue associated to the symmetry, a doubly quantized vortex will be stable. (This is the case in Sec. VII.) We have a local minimum of the Hamiltonian except in the direction of the symmetry. One should notice that this is stability for the doubly quantized vortex against perturbations of the vortex itself, and also against perturbations of the Hamiltonian that preserve the symmetry group G. The choice of Ω has to be made such that it ensures this condition for all m. In this case the system is stable. Otherwise, nonlinear stability is not ensured. The terms that we neglect in the linearization can cause a nonlinear instability if there exist resonance conditions with the negative energy mode. Physically, the picture is that one has a population of quasiparticles which conserves energy.

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linear one and we do not report them here.

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