Vortex Stability Near the Surface of a Bose-Einstein Condensate

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We investigate energetic stability of vortices near the surface of a Bose-Einstein condensate. From an energy functional of a rotating Bose-Einstein condensate, written in terms of variables local to the surface, and a suitable trial wavefunction we calculate the energy of a moving vortex. The energetic stability of the vortex is investigated in terms of the rotation frequency of the confining potential. The critical frequency at which the vortices enter the condensate is calculated and compared with the experiment where a reasonable agreement is obtained.

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I. INTRODUCTION

Since the experimental achievement of Bose-Einstein condensation in confined dilute gases and the observation of vortex lattices [1, 2, 3, 4, 5, 6, 7], much interest has been devoted to the formation, stabilization, and dynamics of vortices [1, 2, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18]. Vortices have been created in Bose-Einstein condensates using two different techniques. The first is a phase imprinting technique [14] and the second is a rotating harmonic trap technique [1, 2, 3, 5, 7]. In the latter technique, a rotating laser beam superposed on the magnetic trap creates an anisotropic confining potential that stirs the condensate. Energetically stable vortices are generated if the rotation frequency \( \Omega \) of the harmonic trap is greater than a certain critical frequency \( \Omega_c \) [16, 19, 20, 24].

As a mechanism for vortex nucleation, it was suggested that vortices are created from the excitation of low-energy surface modes of the Bose-Einstein condensate [17, 21, 22, 23, 24]. For rotational frequencies \( \Omega < \Omega_c \), moving vortices are created in the ultra-dilute region of the condensate. Their effect is observed at the surface of the condensate only as a surface wave [17, 18, 26, 28]. Upon increasing the rotation frequency, the vortices approach the surface of the condensate. At the critical frequency \( \Omega_c \), the vortices enter the condensate, i.e., nucleate. This was supported by Penckwitt et al. [26] with a simulation to the growth of the condensate from a rotating thermal cloud. It was also supported by Anglin [17, 18] who showed, using a boundary layer approach, that the energy barrier to vortex penetration disappears at the Landau critical velocity for surface modes.

This picture for vortex nucleation will be the main focus of the present paper. Using a (rather simple) variational approach to the problem, we investigate the energetic stability of a vortex moving near the surface of the condensate. We verify the above picture by calculating the energy in terms of the distance of the vortex core from the surface \( x_0 \), the rotation frequency \( \Omega \), and the center-of-mass speed of the core of the vortex \( v_0 \). We also calculate the critical frequency \( \Omega_c \) at which the vortex enters the condensate.

In terms of variables local to the surface of large condensates, the surface can be approximated by a plane and the harmonic trapping potential can be approximated by a linear potential [27, 28]. We start by writing the Gross-Pitaevskii energy functional of a rotating condensate in this planar geometry. Using this energy functional with an appropriate trial wavefunction we calculate the energy of a vortex moving in a direction parallel to the surface of the condensate. Then we minimize the energy with respect to the position of the core of the vortex. The resulting equilibrium position of the vortex core is a function of the rotation frequency, the speed of the vortex, and the distance between the vortices in the case when more than a single vortex exists. This allows for a detailed investigation of the stability of the vortex in terms of these parameters.

The rest of the paper is organized as follows. In Sec. 2, we introduce the energy functional of a rotating condensate in the planar geometry. In Sec. 3, we use this energy functional to calculate the energy of a moving vortex as described above. In Sec. 4, we investigate the stability of the vortex in terms of the parameters involved. We end in Sec. 5 by a summary and discussion of our results.

II. ENERGY FUNCTIONAL OF THE SURFACE OF A ROTATING CONDENSATE

In this section we write the Gross-Pitaevskii equation of a rotating condensate in terms of parameters local to the surface of the condensate. Then we construct an energy functional that corresponds to this equation.
The time-dependent Gross-Pitaevskii equation, that describes the behavior of the order parameter $\psi(r,t)$, is given by

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V(r,t) + g|\psi(r,t)|^2 - \mu\right] \psi(r,t) = i\hbar \frac{\partial}{\partial t} \psi(r,t). \quad (1)$$

Here $V(r,t)$ is a time-dependent harmonic trapping potential with time-dependence corresponding to rotating the axes of the trapping potential. The effective two-particle interaction $g$ is proportional to the s-wave scattering length $a$ according to $g = 4\pi a\hbar^2/m$, where $m$ is the mass of an atom, and $\mu$ is the equilibrium chemical potential.

We consider the trap axes in the $x$- and $y$-directions to be rotated counter clockwise around the $z$-axis with angular frequency $\Omega$. The time-dependence of the trapping potential can be removed by writing the Gross-Pitaevskii equation in the following form for the Gross-Pitaevskii equation

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V(r) + g|\psi(r,t)|^2 - \Omega \cdot \mathbf{L} - \mu\right] \psi(r,t) = i\hbar \frac{\partial}{\partial t} \psi(r,t), \quad (2)$$

where $\mathbf{L}$ is the angular momentum operator. The trapping potential, which for simplicity is taken to be isotropic, is given by

$$V(r) = \frac{1}{2}\omega_0^2 r^2, \quad (3)$$

where $\omega_0$ is the characteristic frequency of the trap. Noting that $\Omega \cdot \mathbf{L} = -i\hbar \mathbf{\Omega} \cdot (r \times \nabla) = -i\hbar (\mathbf{\Omega} \times r) \cdot \nabla$, the Gross-Pitaevskii equation takes the form

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V(r) + g|\psi(r,t)|^2 + i\hbar (\mathbf{\Omega} \times r) \cdot \nabla - \mu\right] \psi(r,t) = i\hbar \frac{\partial}{\partial t} \psi(r,t). \quad (4)$$

Next, we express the Gross-Pitaevskii equation in terms of the surface local coordinate $r'$ and surface local velocity $\mathbf{v}'$ via a position transformation

$$r = R\hat{r} + r', \quad (5)$$

where $R = \sqrt{2\mu/m\omega_0^2}$ is the Thomas-Fermi radius of the condensate. The Gross-Pitaevskii equation takes the form

$$\left[-\frac{\hbar^2}{2m} \nabla^2_{r'} + V(R\hat{r} + r') + g|\psi(r',t)|^2 + i\hbar (\mathbf{\Omega} \times r') \cdot \nabla_{r'} + i\hbar (\mathbf{\Omega} \times R\hat{r}) \cdot \nabla_{r'} - \mu\right] \psi(r',t) = i\hbar \frac{\partial}{\partial t} \psi(r',t). \quad (6)$$

The term $i\hbar (\mathbf{\Omega} \times R\hat{r}) \cdot \nabla_{r'}$ can be eliminated by a Galilean transformation to a frame of reference that is moving with a speed $\mathbf{\Omega} \times R\hat{r}$ [20]. Thus, the Gross-Pitaevskii equation becomes

$$\left[-\frac{\hbar^2}{2m} \nabla^2_{r'} + V(R\hat{r} + r') + g|\psi(r',t)|^2 + i\hbar (\mathbf{\Omega} \times r') \cdot \nabla_{r'} - \mu\right] \psi(r',t) = i\hbar \frac{\partial}{\partial t} \psi(r',t). \quad (7)$$

For distances close to the surface of the condensate, such that $r' \ll R$, the trapping potential can be approximated by a linear form as [27]

$$V(R\hat{r} + r') \approx V(R) + \nabla_{r'} V(R\hat{r} + r')_{|r'=0} \cdot r'$$

$$= V(R) + m\omega_0^2 R \hat{r} \cdot r'$$

$$= V(R) + F x, \quad (8)$$

where we have defined the force constant $F = m\omega_0^2 R$ and the surface local coordinate $x = \hat{r} \cdot r'$, which is normal to the surface of the condensate. The coordinates of the $y$ and $z$-components of $r'$ are therefore parallel to the surface. In this plane geometry the Gross-Pitaevskii equation takes the form

$$\left[-\frac{\hbar^2}{2m} \nabla^2_{r'} + \left(F x + g|\psi(r',t)|^2 + i\hbar (\mathbf{\Omega} \times r') \cdot \nabla_{r'}\right)\right] \psi(r',t) = i\hbar \frac{\partial}{\partial t} \psi(r',t). \quad (9)$$

The first and the last terms on the left hand side of this equation can be combined as a complete square, which results in the following form for the Gross-Pitaevskii equation

$$\left[-\frac{\hbar^2}{2m} \left(\nabla_{r'} - \frac{im}{\hbar} \mathbf{\Omega} \times r'\right)^2 + F x + g|\psi(r',t)|^2 - \frac{1}{2}m\left(\mathbf{\Omega} \times r'\right)^2\right] \psi(r',t) = i\hbar \frac{\partial}{\partial t} \psi(r',t). \quad (10)$$
This equation can be derived by differentiating the following lagrangian with respect to $\psi^*(r', t)$

$$L[\psi, \psi^*] = \int dr' \left( \frac{i\hbar}{2} \left( \psi^* \frac{\partial \psi}{\partial t} - \psi \frac{\partial \psi^*}{\partial t} \right) - E[\psi, \psi^*] \right),$$

where $E[\psi, \psi^*]$ is given by

$$E[\psi, \psi^*] = \int dr' \left[ \frac{\hbar^2}{2m} \left( \nabla_{r'} - \frac{i m}{\hbar} \Omega \times r' \right) \psi(r', t) \right]^2 + F x |\psi(r', t)|^2 + \frac{1}{2} g |\psi(r', t)|^4 - \frac{1}{2} m (\Omega \times r')^2 |\psi(r', t)|^2 \right].$$

### III. ENERGY OF A MOVING VORTEX NEAR THE SURFACE OF THE CONDENSATE

We consider a vortex with axis parallel to the surface of the condensate, say parallel to the $z$-direction. The core of the vortex is located at a distance $x = x_0$ from the Thomas-Fermi surface of the condensate and is moving in the positive $y$-direction with a speed $v_0$. This is depicted in the schematic figure Fig. 1. For simplicity, we consider a vortex with a small core size such that the equilibrium condensate density can be considered constant over distances of the order of the core size.

The normalized density profile of the vortex is given by $\chi^2(x - x_0, y - v_0 t)$, where we assume for $\chi(x - x_0, y - v_0 t)$ the trial function

$$\chi^2(x - x_0, y - v_0 t) = \sqrt{\frac{\rho}{2\xi^2 + \rho^2}},$$

whith $\rho = \sqrt{(x - x_0)^2 + (y - v_0 t)^2}$, and $\xi = 1/\sqrt{8\pi n_0(x_0)}$ is the coherence length of the condensate calculated at $x_0$. 

![Figure 1](image_url)
The phase of the vortex $\Phi(x - x_0, y - v_0 t)$ must satisfy
\[
\frac{\hbar}{m} \nabla_r \Phi = \frac{\hbar}{m \rho} \Phi + v_0 \hat{y}
\]
\[
= \frac{\hbar}{m \rho} \cos \phi \hat{x} + (v_0 - \frac{\hbar}{m \rho} \sin \phi) \hat{y},
\]
where $\rho$ and $\phi$ are the polar coordinates in the $x$-$y$ plane with the origin being at the core of the vortex as shown in Fig. 1. This equation expresses the fact that the velocity has two components: the superfluid velocity $\overline{v}_f/m \rho$ associated with the vortex, and the center-of-mass velocity $v_0 \hat{y}$.

In Appendix A, we show that using the trial function Eq. (13) in the energy functional Eq. (12), the energy of the vortex per unit length along the axis of the vortex takes the form
\[
E = n_0(x_0) \int d\rho \left[ \frac{\hbar^2}{2m} \left( (\nabla \chi)^2 + \frac{\chi^2}{\rho^2} \right) + \frac{1}{2} \nu n_0(x_0) \chi^4 \right]
+ n_0(x_0) \left[ \frac{1}{2} m v_0^2 + \hbar \Omega - m \Omega x_0 v_0 + F x_0 \right] \int d\rho \chi^2.
\]

The quantity of interest is the extra energy associated with the presence of the vortex [31]. Therefore, we have to subtract the vortex energy given by the last equation from the energy of a vortex-free system that contains the same number of atoms as the system with the vortex. The energy density of the vortex-free system is only that of the mean-field interaction, the trapping potential, and the energy associated with the rotation, namely
\[
E_{vf} = \frac{1}{2} g \rho_0^2 n_0(x_0) + F x_0 n_0(x_0) + \hbar \Omega n_0(x_0),
\]
where the subscript “vf” in $E_{vf}$ denotes vortex free. To fulfill the requirement that the number of atoms $\nu$ in both systems must be the same, we calculate the energy of both systems within a cylindrical region of axis normal to the $x$-$y$ plane and circular cross-section of radius $b$. The radius $b$ must be, on the one hand, larger than several coherence lengths $\xi$ in order to incorporate all density variations associated with the presence of the vortex. On the other hand, $b$ must be much smaller than the length over which the density changes significantly in order not to violate the local-density approximation used to derive calculate the energies Eqs. (17) and (18). The number of atoms per unit length of the axis of the cylinder in the system that contains the vortex can be expressed as
\[
\nu = n_0(x_0) \int_0^b 2\pi \rho d\rho \chi^2
= \pi b^2 n_0(x_0) - n_0(x_0) \int_0^b 2\pi \rho d\rho (1 - \chi^2).
\]

Using this number to calculate the average density as $n_0(x_0) = \nu^2/\pi b^2$, the energy per unit length of the vortex-free system is given by
\[
E_{vf} \simeq \frac{1}{2} \pi b^2 g \rho_0^2 n_0(x_0) - g \rho_0^2 n_0(x_0) \int_0^b 2\pi \rho d\rho (1 - \chi^2) + (F x_0 n_0(x_0) + \hbar \Omega n_0(x_0)) \int 2\pi \rho d\rho \chi^2.
\]

In this equation we ignore terms that are second order in $1 - \chi^2$ in the mean-field energy [31].

Subtracting Eq. (20) from Eq. (17), we obtain the energy associated with the presence of the vortex per unit length of its axis:
\[
E_v = n_0(x_0) \int d\rho \left[ \frac{\hbar^2}{2m} \left( (\nabla \chi)^2 + \frac{\chi^2}{\rho^2} \right) + \frac{1}{2} g n_0(x_0) (\chi^2 - 1)^2 \right]
+ n_0(x_0) \left[ \frac{1}{2} m v_0^2 - m \Omega x_0 v_0 \right] \int d\rho \chi^2 + \hbar \Omega \int d\rho (\chi^2 - 1) + F x_0 n_0(x_0) \int d\rho (\chi^2 - 1).
\]

We recognize the first line of this equation as the internal energy of the vortex [31].
IV. STABILITY ANALYSIS

In this section we consider an infinite string of equidistant moving vortices. The string is parallel to the surface of the condensate, say along the y-axis, and the vortices move in that direction with a constant speed \( v_0 \). The distance between two adjacent vortices \( \lambda \) is large enough such that the cores do not overlap. In this case, the energy of the string of vortices per unit length of the string is just the energy of one vortex given by Eq. (21) times the number of vortices per unit length. Therefore, it is sufficient to perform the analysis by calculating the energy of a single vortex.

This energy will be a function of \( \lambda \) that corresponds to a certain number of vortices per unit length.

In the following, we investigate the dependence of the equilibrium position of the vortex on the rotation frequency \( \Omega \), the distance between two adjacent vortices \( \lambda \), and the vortex speed \( v_0 \).

For convenience, we rewrite Eq. (21) in terms of scaled quantities as follows:

\[
\tilde{E}_v = \tilde{c}_v + \nu_1 \tilde{n}_0(\tilde{x}_0)(\tilde{\rho}^2 - 2\tilde{\Omega} \tilde{x}_0 \tilde{v}_0) + \nu_2 \tilde{n}_0(\tilde{x}_0)(2\tilde{\Omega} + \tilde{x}_0),
\]

where \( \nu_1 = 2\pi \int_0^b \tilde{\rho} d\tilde{\rho} \tilde{\chi}^2 \), \( \nu_2 = 2\pi \int_0^b \tilde{\rho} d\tilde{\rho} (\tilde{\chi}^2 - 1) \), and

\[
\tilde{c}_v = 2\pi \tilde{n}_0(\tilde{x}_0) \int_0^b \tilde{\rho} d\tilde{\rho} \left[ \left( \nabla \tilde{\chi} \right)^2 + \frac{\chi^2}{\tilde{\rho}^2} \right] + \frac{1}{2} \tilde{n}_0(\tilde{x}_0)(\tilde{\chi}^2 - 1)^2
\]

is the internal energy of the vortex. Here, the gradient operator is with respect to \( \tilde{\rho} \). Length is scaled to the characteristic length at the surface of the condensate \( \delta \) defined by \( \hbar^2/2m\delta^2 = F\delta \). The vortex velocity \( v_0 \) is scaled to \( \hbar/m\delta \), the angular frequency \( \Omega \) is scaled to \( \hbar/m\delta^2 \), the density \( n_0 \) is scaled to \( 8\pi a\delta^2 \), and the energies \( E_v \) and \( c_v \) are scaled to \( (\hbar^2/2m\delta^2)/(8\pi a/\delta) = ((2R/a_0)^{1/3}/16\pi)\hbar\omega_0 \). In these dimensionless variables, Eq. (14), takes the form

\[
-\frac{d^2}{dx^2} + \tilde{x} + \tilde{n}_0(\tilde{x}_0) \sqrt{\tilde{n}_0(\tilde{x}_0)} = 0.
\]

Furthermore, the vortex profile \( \chi \), defined in Eq. (15), takes the form

\[
\chi = \frac{\tilde{\rho}}{\sqrt{2/\tilde{n}_0(\tilde{x}_0) + \tilde{\rho}^2}}.
\]

Since the distance between two adjacent vortices is \( \tilde{\lambda} \), the upper limit of the integrations in the expressions for \( \nu_1, \nu_2 \), and Eq. (23) is taken as \( b = \lambda/2 \).

We start by minimizing the vortex energy \( \tilde{E}_v \) with respect to the vortex linear speed \( \tilde{v}_0 \). This gives simply \( \tilde{v}_0 = \tilde{x}_0 \tilde{\Omega} \), which is similar to the relation between the center of mass speed and the angular frequency of a rolling rigid wheel of radius \( \tilde{x}_0 \). Substituting this value for \( \tilde{v}_0 \) in Eq. (22), the energy of the vortex becomes

\[
\tilde{E}_v = c_v - \nu_1 \tilde{n}_0(\tilde{x}_0) \tilde{x}_0^2 \tilde{\Omega}^2 + \nu_2 \tilde{n}_0(\tilde{x}_0)(2\tilde{\Omega} + \tilde{x}_0).
\]

The equilibrium position of the vortex \( \tilde{x}_{eq} \) is obtained by minimizing the energy \( \tilde{E}_v \) with respect to the vortex distance from the surface \( \tilde{x}_0 \), for a given set of the parameters \( \tilde{\Omega} \) and \( \tilde{\lambda} \). The main focus will be on the behavior of the equilibrium position \( \tilde{x}_{eq} \) as a function of the parameters \( \tilde{\Omega} \) and \( \tilde{\Lambda} \). In particular, we are interested in situations when the vortex enters the condensate. The Thomas-Fermi surface, defined by \( \tilde{x}_0 = 0 \), is to be taken as the boundary for considering the vortices inside or outside the condensate. Vortices located in the region \( \tilde{x}_0 > 0 \) are to be considered out of the condensate, while those in the region \( \tilde{x}_0 < 0 \) are considered inside the condensate.

To calculate the vortex energy \( \tilde{E}_v \), we first need to solve Eq. (24) for \( \tilde{n}_0(\tilde{x}_0) \). As a first approximation we use the Thomas-Fermi approximation for the condensate density \( \tilde{n}_0(\tilde{x}_0) \). This is obtained by neglecting the first term in Eq. (24), namely

\[
\tilde{n}_0(\tilde{x}_0) = \begin{cases} 
-\tilde{x}_0, & \tilde{x}_0 < 0 \\
0, & \tilde{x}_0 > 0
\end{cases}
\]

The Thomas-Fermi approximation is accurate only in the deep region of the condensate \( \tilde{x}_0 \ll 0 \). Thus, the results we obtain here using this approximation will be accurate only in that region. From Eq. (26) we see that the core size of the vortex depends on the condensate density. This will complicate the dependence of the energy on the vortex location. For simplicity, we take the size of the core to be constant and is equal to its value at the Thomas-Fermi
surface. Substituting for \( \tilde{n}_0(\tilde{x}_0) \) from Eq. (27) in Eq. (26), the vortex energy \( \tilde{E}_v \) becomes a cubic function in \( \tilde{x}_0 \), which can be written as

\[
\tilde{E}_v = -(\alpha_1 + 2\tilde{\Omega}v_2)\tilde{x}_0 + (\alpha_2 - \nu_2)\tilde{x}_0^2 + \nu_1\tilde{\Omega}^2\tilde{x}_0^3
\]

(28)

where

\[
\alpha_1 = 2\pi \int_0^{\tilde{b}} \tilde{\rho}d\tilde{\rho} \left( (\nabla\chi)^2 + \chi^2 \right),
\]

(29)

and

\[
\alpha_2 = 2\pi \int_0^{\tilde{b}} \tilde{\rho}d\tilde{\rho} \frac{1}{2}(\chi^2 - 1)^2.
\]

(30)

To be able to extract the main features of this energy expression, we point out some properties of the numbers \( \nu_1 \) and \( \nu_2 \) and the parameters \( \alpha_1 \) and \( \alpha_2 \). The number \( \nu_1 \) is always positive since it corresponds to the number of atoms within a circle of radius \( \tilde{b} \) centered at the axis of a vortex that is embedded in a uniform background of density \( \tilde{n}_0 = 1 \). The number \( \nu_2 \) is always negative since it is the difference between the number of atoms in the vortex and the number of atoms in a vortex-free background. The parameter \( \alpha_1 \) corresponds to the kinetic energy due to the gradient of the wavefunction of the vortex. The parameter \( \alpha_2 \) corresponds to the mean-field interaction energy. It should be also noted that Eq. (28) is defined only for negative values of \( \tilde{x}_0 \).

With this in mind, we conclude from Eq. (28) that \( \tilde{E}_v \) starts linearly for small \( \tilde{x}_0 \) with a slope \( -(\alpha_1 + 2\tilde{\Omega}v_2) \) that, depending on the value of \( \tilde{\Omega} \), can be either positive or negative. For large \( \tilde{x}_0 \), the energy \( \tilde{E}_v \) behaves as \( \nu_1\tilde{\Omega}^2\tilde{x}_0^3 \) which is large and negative. If the initial slope \( -(\alpha_1 + 2\tilde{\Omega}v_2) \) is positive, \( \tilde{E}_v \) will have only a local maximum at some value of \( \tilde{x}_0 \). If, on the other hand, the slope is negative, \( \tilde{E}_v \) may have a local minimum in addition to a local maximum. If the negative value of the slope is large enough, the value of \( \tilde{E}_v \) at the local maximum can vanish or even disappear. To be more explicit, we rewrite Eq. (28) as

\[
\tilde{E}_v = \tilde{x}_0 [(\tilde{x}_0 - x_1)(\tilde{x}_0 - x_2)],
\]

(31)

where

\[
x_1 = \frac{-\alpha_2 - \nu_2}{2\nu_1\tilde{\Omega}^2} + \frac{1}{2\nu_1\tilde{\Omega}^2}\sqrt{(\alpha_2 - \nu_2)^2 + 4\nu_1\tilde{\Omega}^2(\alpha_1 + 2\nu_2\tilde{\Omega})},
\]

(32)

and

\[
x_2 = \frac{-\alpha_2 - \nu_2}{2\nu_1\tilde{\Omega}^2} - \frac{1}{2\nu_1\tilde{\Omega}^2}\sqrt{(\alpha_2 - \nu_2)^2 + 4\nu_1\tilde{\Omega}^2(\alpha_1 + 2\nu_2\tilde{\Omega})},
\]

(33)

are two of the three roots of Eq. (31). The value of \( \tilde{E}_v \) at the local maximum vanishes when \( x_1 = x_2 \). This can be satisfied if

\[
(\alpha_2 - \nu_2)^2 + 4\nu_1\tilde{\Omega}^2(\alpha_1 + 2\nu_2\tilde{\Omega}) = 0,
\]

(34)

which is the condition that gives the critical frequency \( \tilde{\Omega}_c \) at which the height of the energy barrier for vortex nucleation vanishes.

The expression for \( \tilde{E}_v \) is plotted in Fig. 2 as a function of \( \tilde{x}_0 \) for different values of \( \tilde{\Omega} \) and one value of \( \tilde{\lambda} \). In addition to the above-mentioned properties of the energy curve, the figure shows that the height of the barrier decreases with increasing \( \tilde{\Omega} \). At a certain value of \( \tilde{\Omega} \) the height of the barrier vanishes and the vortex can enter the condensate. For the value of \( \tilde{\lambda} \) used in this figure, we find that, at \( \tilde{\Omega} = 0.5 \), the height of the barrier vanishes. This critical value of \( \tilde{\Omega} \) is indeed equal to the real root of Eq. (31).

Since the Thomas-Fermi approximation, used here, is not accurate at the surface, we will not attempt to calculate the critical frequency at which the vortex enters the condensate. This is to be investigated next where we use the exact density profile of the condensate.

For a more accurate treatment of the problem, we repeat the above calculation using the numerical solution of Eq. (24) instead of the Thomas-Fermi one. We start by solving numerically Eq. (24) for \( \tilde{n}_0(\tilde{x}_0) \), and then using this result in Eq. (25) to calculate \( \chi \), where the coherence length \( \xi \) depends on \( \tilde{n}_0(\tilde{x}_0) \) and is not taken to be constant as in the above calculation. These values of \( \tilde{n}_0(\tilde{x}_0) \) and \( \chi \) are then used to calculate \( \tilde{E}_v \) from Eq. (25).
FIG. 2: Vortex energy $\tilde{E}_v$ as a function of the distance between the core of the vortex and the Thomas-Fermi surface $\tilde{x}_0$. The energy is calculated using the Thomas-Fermi approximation. Five curves are plotted for values of $\tilde{\Omega}$ that equal, starting from the uppermost curve, 0.1, 0.45, 0.5, 0.55, 0.6. The value of $\tilde{\lambda}$ used is 21. The unit of energy is $((2R/a_0)^{1/3}/16\pi)\bar{h}\omega_0$ and the unit of distance is $\delta$. For a typical experiment such as the one discussed at the end of Sec. IV, the unit of energy equals $0.033\bar{h}\omega_0$, and the unit of distance equals $0.6a_0$, where $a_0 = \sqrt{\hbar/m\omega_0}$.

FIG. 3: Vortex energy $\tilde{E}_v$ as a function of the distance between the core of the vortex and the Thomas-Fermi surface $\tilde{x}_0$. The energy is calculated numerically. Five curves are plotted for values of $\tilde{\Omega}$ that equal, starting from the uppermost curve, 0.0, 0.17, 0.34, 0.51, 0.68. The value of $\tilde{\lambda}$ used is 21. Note that the height of the energy barrier vanishes for $\tilde{\Omega} = 0.34$.

result obtained using the Thomas-Fermi approximation, we find that $\tilde{E}_v$ has a local minimum and a local maximum, and tends to $-\infty$ as $\tilde{x}_0 \to -\infty$. In Fig. 3 we plot the energy $\tilde{E}_v$ as a function of $\tilde{x}_0$ for different values of $\tilde{\Omega}$. This figure is to be compared with Fig. 4 of Ref. [18] and Fig. 5 of Ref. [13]. The main feature of Figs. 2 and 3, which is that an energy barrier for vortex nucleation exists and that the height of the barrier decreases with increasing $\tilde{\Omega}$, agrees with the above-mentioned two figures. However, a detailed comparison is not possible for the following reasons. In Fig. 4 of Ref. [18] the energy is calculated in the outer region of the condensate, which means that it is accurate only for large distances away from the Thomas-Fermi surface. In Fig. 5 of Ref. [13] the energy is calculated using the Thomas-Fermi approximation and therefore is accurate only inside the condensate. The present calculation is valid in the region near the surface of the condensate from both sides. Thus, Fig. 3 presents a calculation of the energy in a region where both calculations of Refs. [18] and [13] are not applicable.

In Fig. 4 we plot the position of the local minimum of the energy and the height of the energy barrier as a function of $\tilde{\Omega}$. Several curves are plotted corresponding to different values of $\tilde{\lambda}$. Fig. 4(a) shows that the vortex approaches the surface when $\tilde{\Omega}$ is increased. To enter the condensate, the energy barrier has to vanish. Fig. 4(b) shows that the energy barrier does indeed vanish for a certain value of $\tilde{\Omega}$. This value is to be considered as the critical value $\tilde{\Omega}_c$ at which the vortex nucleates.

Now, we can compare our predictions for the critical frequency at which the vortex nucleates with those observed experimentally. To that end, we need to express $\tilde{\Omega}_c$ in terms of the harmonic trap frequency $\omega_0$ for a spherical condensate. This is readily obtained by noticing that the characteristic length scale at the surface of the condensate $\delta$ is related to the Thomas-Fermi radius of the condensate through $\delta = (\hbar^2/2mF)^{1/3} = (a_0/2R)^{1/3}a_0$, where $a_0 = \sqrt{\hbar/m\omega_0}$. Using this relation, $\tilde{\Omega}$ can be expressed in terms of $\omega_0$ as $\tilde{\Omega} = (\Omega/\omega_0)(a_0/2R)^{2/3}$, which simply leads to
FIG. 4: a) The equilibrium position of the vortex core versus the rotation frequency of the magnetic trap. These curves are calculated for values of $\tilde{\lambda}$ that equal, starting from the lowest curve, 10, 12, 14, 16, 18, 20. The sudden drop in two of the curves appear because the local minimum of $\tilde{E}_v$ is no longer present. The local minimum and local maximum merge to form a stationary point. b) The height of the energy barrier calculated for values of $\tilde{\lambda}$ that equal, starting from the rightmost curve, 10, 12, 14, 16, 18, 20. The units of energy and distance are as those mentioned in Fig. 2, and the unit of frequency is $(2R/a_0)^{2/3}\omega_0$, which for the experiment discussed at the end of Sec. IV equals $2.6\omega_0$.

$$\Omega = (2R/a_0)^{2/3}\tilde{\Omega}\omega_0.$$  

In the experiment of the ENS group [1], a single vortex was created in about $1 \times 10^5$ atoms of a $^{87}$Rb condensate at a rotating frequency $\Omega = 2\pi \times 147$ Hz. The magnetic trap used was axially symmetric with axial trap frequency $\omega_z = 2\pi \times 11.7$ Hz and radial trap frequency $\omega_\perp = 2\pi \times 219$ Hz. The scattering length is taken as $a = 5.8$nm. For these parameters $R \approx 2.1a_0$ and $(2R/a_0)^{2/3} \approx 2.6$, where we have used $a_0 = (\hbar/m(\omega_\perp^2\omega_z)^{1/3})^{1/2}$. For a single vortex the value of $b$ is half the circumference of the condensate, namely $b \approx 2.1\pi a_0 \approx 10.5\delta$. Since $\tilde{\lambda} = 2\tilde{b}$, the lowest curve of Fig. 4(a) and the left most curve of Fig. 4(b) correspond to the case of a single vortex. For the latter curve the height of the barrier vanishes at $\tilde{\Omega}_c \approx 0.34$. (Notice that this corresponds to the number obtained above using the Thomas-Fermi approximation, namely $\tilde{\Omega}_c \approx 0.5$). Thus, according to our calculation, the critical frequency for vortex nucleation is $\Omega_c/\omega_0 = 0.88$. This is to be compared with the experimental number $\Omega_c/\omega_\perp = 147/219 = 0.68$. Notice that we consider $\omega_0$ to correspond to $\omega_\perp$ since in the experiment the axis of rotation is the $z$-axis. Taking into account the approximations that we have used, we consider this agreement to be reasonable. One possible reason for the disagreement is that we have taken the core of the vortex to be small compared to the distance over which the density of the condensate changes significantly. This approximation is accurate only in the deep region of the condensate and not close to the Thomas-Fermi surface or away from it. Furthermore, our criterion for vortex nucleation may be too restrictive since, even with a nonzero barrier height, as shown in Fig. 4(b), the vortex can tunnel through the barrier and thus nucleate at a frequency which is less than that obtained above.

V. CONCLUSION

We have written down the energy functional of a rotating Bose-Einstein condensate in terms of variables local to its surface. Using a variational ansatz, we have calculated the energy of a single vortex moving at the surface of the condensate. This energy was used to investigate the energetic stability of the vortex in terms of the rotation frequency of the confining potential. Upon increasing the rotation frequency, the vortex approaches the surface of the
condensate. At a critical rotation frequency, the vortex crosses the surface of the condensate and enters it.

The local-density approximation was used to simplify the calculations and lead to analytical results in the Thomas-Fermi limit. This approximation is accurate only in the interior of the condensate and not near the Thomas-Fermi surface or away from it. The critical frequency obtained using this approximation is thus not expected to be accurate. Therefore, we solve the problem numerically including kinetic energy effects at the surface. This leads to more accurate values for the critical frequency that compare reasonably with experiment. It should be also noted that our criterion for vortex nucleation, which is requiring that the energy barrier vanish, may be too restrictive. When the height of the energy barrier is nonzero but small enough, the vortex can tunnel through it and thus nucleate at a rotation frequency that is less than the one we calculated in the previous section. In this sense, our calculated critical frequency may be regarded as an upper bound to the vortex nucleation frequency.

APPENDIX A: DETAILS OF THE ENERGY CALCULATION

In this Appendix we present details for the derivation of Eq. (17) from the energy functional Eq. (12) using the trial wave function Eq. (13) for a moving vortex.

Since the vortex axis is parallel to the $z$-axis and the vortex is moving in the $y$-direction, the nontrivial contributions to the energy arise only from integrating over $x$ and $y$. Therefore, we calculate the energy of the vortex per unit length of the $z$-direction, which means that we have to perform only integrals in the $x$-$y$ plane. It is, thus convenient to shift the origin of $\mathbf{r}'$ from the surface of the condensate to the core of the vortex and to express the integral of energy functional in the polar coordinates $\rho$ and $\phi$. Explicitly, we make the transformation $\mathbf{r}' = x_0 \hat{x} + \rho$.

The kinetic energy contribution reads

$$E_k = \int d\rho \frac{\hbar^2}{2m} \left| \left( \nabla - \frac{im}{\hbar} \Omega \times (x_0 \hat{x} + \rho) \right) \psi(\rho, \phi) \right|^2,$$

where, here and through out this appendix, the gradient term is with respect to $\rho$. Inserting the trial function Eq. (13) in this equation we obtain

$$E_k \simeq \frac{\hbar^2}{2m} n_0(x_0) \int d\rho \left| \left( \nabla - \frac{im}{\hbar} \Omega \times (x_0 \hat{x} + \rho) \right) \chi(\rho) \exp \left( i \Phi(\rho) \right) \right|^2.$$  \hspace{1cm} (A2)

Here, we have employed the approximation that the condensate equilibrium density $n_0(x)$ is constant over distances of the order of the coherence length. For this approximation to be valid, the upper limit of the integration over $\rho$ must be much less than the distance over which the condensate density changes significantly. In this case we can approximate $n_0(x)$ by its value at $x_0$ and take it out of the integration. Furthermore, the last equation can be simplified to

$$E_k = \frac{\hbar^2}{2m} n_0(x_0) \int d\rho \left| \nabla \chi + i \chi \nabla \Phi - \frac{im}{\hbar} \Omega \times (x_0 \hat{x} + \rho) \chi \right|^2$$

$$= \frac{\hbar^2}{2m} n_0(x_0) \int d\rho \left[ (\nabla \chi)^2 + (\chi \nabla \Phi)^2 + \frac{m^2}{\hbar^2} (\Omega \times (x_0 \hat{x} + \rho))^2 \chi^2 - 2 \frac{m}{\hbar} (\Omega \times (x_0 \hat{x} + \rho) \cdot \nabla \Phi) \chi \right].$$  \hspace{1cm} (A3)

Knowing that $\Omega = \Omega \hat{x}$ and using the expression for $\Phi$ from Eq. (16), it is straightforward to show that the kinetic energy takes the form

$$E_k = \frac{\hbar^2}{2m} n_0(x_0) \int d\rho \left[ (\nabla \chi)^2 + \frac{\chi^2}{\rho^2} + \frac{m^2 v_0^2}{\hbar^2} \chi^2 + \frac{2m}{\hbar} \Omega (1 - \frac{m}{\hbar} x_0 v_0) \chi^2 + \frac{m^2}{\hbar^2} \Omega^2 (x_0^2 + \rho^2) \chi^2 \right].$$  \hspace{1cm} (A4)

The contribution to the energy from the last term of Eq. (12) is

$$E_{\Omega} = - \frac{1}{2} m n_0(x_0) \int d\rho (\Omega \times (x_0 \hat{x} + \rho))^2 \chi^2$$

$$= - \frac{1}{2} m \Omega^2 n_0(x_0) \int d\rho (x_0^2 + \rho^2) \chi^2.$$  \hspace{1cm} (A5)

When added to the kinetic energy, this term cancels with the last term of Eq. (A4).
The contribution of the external trapping potential is given by

\[ E_{\text{ext}} = F n_0(x_0) \int d\rho(x_0 + \rho \sin \phi) \chi^2 \]

\[ = F n_0(x_0) x_0 \int d\rho \chi^2. \]  

(A6)

The contribution of the interatomic interaction reads simply

\[ E_{\text{int}} = \frac{1}{2} g n_0^2(x_0) \int d\rho \chi^4. \]  

(A7)

Finally, we add all these contributions to obtain Eq. (17).

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