

Metastable off-axis vortices in nonrotating Bose-Einstein condensates

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Abstract. We propose a scenario for studying vortices confined by nonrotating traps. For this purpose we model a polynomial trapping potential that can sustain locally stable off-axis vortices. We also describe a simple numerical method for generating vortices without relying on rotating frames or centrifugal potential techniques. This method offers other advantages related to the control in the number of vortices to be generated and in their location. Finally, we compute the vortex energy as a function of its position using three approaches and discuss their validity. We show that a well defined energy barrier between the vortex and the ground state is obtained.

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1. Introduction

Quantized vortices arise as striking topological defects yielding one of the most important signatures of superfluidity [1]. In the last decade, in trapped Bose-Einstein condensates (BECs), an enormous amount of work, both theoretical and experimental, has been devoted to studying the structure, stability and dynamics of vortices (For a review of these issues, see, for example [2–4]).

Since vortices in BECs were first experimentally produced by Matthews *et al.* [5], many techniques were developed for their generation. Among the most ingenious ones, we can quote that vortex rings have been obtained as a result of the decay of solitons [6]. Vortex lines have been generated from the application of topological phase imprinting methods [7]. And finally, a large variety of configurations, from single vortex to vortex lattices, are being generated using rotating traps [8–10]. In connection to vortex instabilities, the decay of a doubly quantized vortex into two singly quantized vortices has been observed [11]. In recent experiments, alternative trapping potentials, quadratic plus quartic polynomial, have been constructed in order to obtain vortex lattices in fast rotating condensates [9, 10]. The quartic term in the potential has been introduced to stabilize the system when the angular velocity exceeds the radial angular frequency of the quadratic term [12, 13].

From a theoretical point of view the numerical generation of stationary vortices has not been an easy task. In rotating condensates, energetically stable vortices have been obtained by minimizing their energy as described in the rotating frame (see [2–4] and references therein). This method usually requires a large number of iterations because the vortices are dragged from the border of the condensate making difficult to control the number and location of the vortices to be generated. On the other hand, in nonrotating condensates, structural and dynamically stable, yet energetically unstable vortices, have been created by several techniques [14–16]. These vortices cannot be found with the usual methods based on energy minimization and thus, for example in Ref. [16] the solutions were obtained by minimizing a specially constructed error functional. The standard nonrotating Bose-Einstein condensate has a parabolic profile, which is obtained with an harmonic oscillator confinement. A characteristic of the parabolic profile is that in the presence of dissipation an off-axis vortex spirals away from the condensate. As far as we know, the problem of finding a family of nonrotating lowest-order polynomial trapping potential that can sustain metastable off-axis vortices within a BEC has not been addressed. Note that only local stability may be achieved because the ground state has a lower energy. Depending on the form of the energy barrier between the vortex and the ground state a persistent current may survive even in presence of a thermal cloud and therefore we believe this problem may be interesting from a fundamental perspective. Hereafter when we refer to stable vortices we will be meaning locally stable ones.

Finally, we want to mention that exploratory and stimulating analytical work has been devoted to the study of the dynamics of vortices in spatially inhomogeneous two-

dimensional superfluids [17–22]. We believe it would be interesting to extend these studies and perform numerical calculations with more general types of density profiles than the parabolic one.

Therefore, in this work we present a fourth-order polynomial trapping potential that can sustain off-axis vortices, and describe a simple numerical phase imprinting (NPI) method for obtaining such states. With this trap the system exhibits a vortex energy barrier near the border of the condensate. As the stability of the vortex in presence of dissipative processes is related to the shape of this energy barrier, we find convenient to compute it using different approaches. Also it is important for describing, for example, quantum tunneling processes.

The work is organized as follows. In section 2 we describe the system and the proposed trapping potential. In section 3 we explain the NPI method for numerically producing vortices in absence of rotating frames. In section 4 we introduce an approximate expression with a single fitting parameter for the vortex energy, and in section 5 we present numerical calculations of the vortex energy employing different approaches. Finally, the summary and concluding remarks are offered in section 6.

2. The trapping potential

We consider a Bose-Einstein condensate of atoms confined by an external trap V_{trap} . The Gross-Pitaevskii (GP) energy density functional for the system at zero temperature has the standard form

$$E[\psi] = \int \left(\frac{\hbar^2}{2m} |\nabla \psi|^2 + V_{\text{trap}} |\psi|^2 + \frac{1}{2} g |\psi|^4 \right) d^3r, \quad (1)$$

where ψ is the condensate wave function and m is the atom mass. The coupling constant g is written in terms of the s -wave scattering length a as $g = 4\pi a \hbar^2 / m$.

Variation of E with respect to ψ keeping the number of particles, N , fixed yields the GP equation

$$\left(-\frac{\hbar^2 \nabla^2}{2m} + V_{\text{trap}} + g |\psi|^2 \right) \psi = \mu \psi, \quad (2)$$

where μ is the chemical potential.

We mathematically model a polynomial trapping potential, which written in cylindrical coordinates reads

$$V_{\text{trap}}(r, z) = \frac{1}{2} m \left[\omega_r^2 \frac{r^2 (r - r_1) (r - r_2)}{r_1 r_2} + \omega_z^2 z^2 \right], \quad (3)$$

where ω_r and ω_z are radial and axial angular frequencies, respectively. As a function of r this trapping potential has two zeroes at r_1 and r_2 , a local maximum at $R_- < r_1$, and two local minima at $r = 0$ and R_+ with $r_1 < R_+ < r_2$. The local extrema at R_{\mp} are given by

$$R_{\mp} = \frac{3(r_1 + r_2) \mp \sqrt{9(r_1 - r_2)^2 + 4r_1 r_2}}{8}. \quad (4)$$

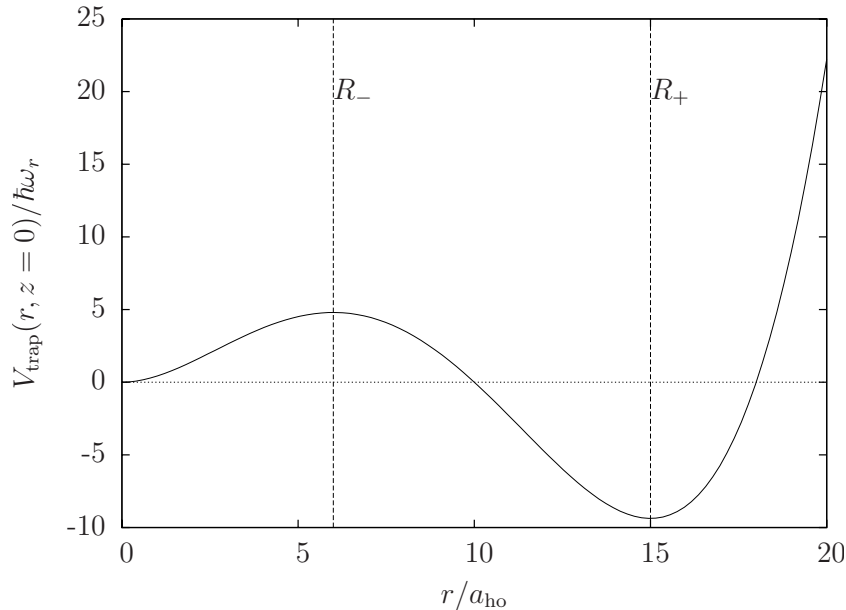


Figure 1. Trapping potential V_{trap} (in units of $\hbar\omega_r$) as a function of r at $z = 0$ (in units of $a_{\text{ho}} = \sqrt{\hbar/(m\omega_r)}$).

The minimum of the potential at R_+ gives rise to a maximum in the ground state density that, as we shall see, generates a vortex-energy barrier, which prevents the vortex to spiral away from the condensate. On the other hand, the local potential maximum generates a local minimum in the density of particles, which in turn should yield a local minimum of the vortex energy.

In figure 1 we show the trapping potential for $(r_1, r_2) = (10, 18)$, in units of $a_{\text{ho}} = \sqrt{\hbar/(m\omega_r)}$. Hereafter we shall always use a_{ho} as the unit of length. For this set of parameters the extrema are located at $R_- = 6$ and $R_+ = 15$.

We consider a system formed by $N = 10^6$ atoms of ^{87}Rb whose scattering length is $a = 98.98a_0$, where a_0 is the Bohr radius. We have chosen $\omega_r/(2\pi) = 100$ Hz and $\omega_z/(2\pi) = 520$ Hz, in order to obtain a pancake-shaped condensate. In figure 2 we show the ground-state density $\rho = |\psi_0|^2$ as a function of x at $y = 0$ and $z = 0$, which was obtained by solving the GP equation.

The number of particles is large enough to assume that the condensate in the (x, y) plane is in the Thomas-Fermi (TF) regime. In this situation one can obtain the density of the ground state using (2) neglecting the kinetic term as

$$|\psi_0(r, 0)|^2 = \frac{1}{g} [\mu - V_{\text{trap}}(r, 0)] \Theta [\mu - V_{\text{trap}}], \quad (5)$$

where Θ is the Heaviside function. It may be observed that the shape of the density profile depicted in figure 2 corresponds to the inverted potential as predicted by the TF approximation.

Depending on the values of r_1 and r_2 , one can model different shapes of densities, and thereby change the position of the critical points, R_- and R_+ , and the height of the vortex energy barrier. We want to mention that, in a recent work, Cozzini *et al.* [23]

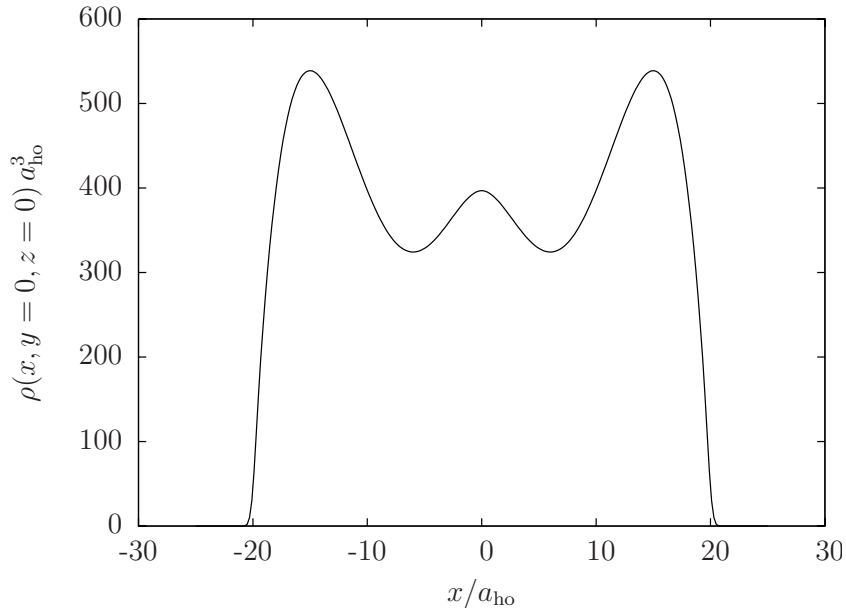


Figure 2. Ground-state density profile ρ for $y = 0$ and $z = 0$ as a function of x for $(r_1, r_2) = (10, 18)$.

have considered an harmonic-plus-quartic trapping potential that also exhibits local extremes with the relative maximum located at $R_- = 0$.

3. The numerical phase imprinting method

In this section we describe a numerical method to generate a stationary vortex state that is a local minimum of the energy functional. The method consists in the choice of an initial guess for the wavefunction and the subsequent minimization of the energy (1). Due to their simplicity we have adopted two standard methods that directly minimize the energy, namely, an evolution of the wavefunction in imaginary time [24] and a conjugate gradients technique [25]. For the singly quantized vortex we have found that both methods work satisfactorily and produce the same results; however, as the conjugate gradient method usually requires less time to converge to a desired accuracy we present the results obtained with that method only.

As the starting point of the minimization, we choose a smooth real function $\psi_0(\mathbf{r})$, preferably the ground-state wavefunction, and construct the initial state as

$$\psi'(\mathbf{r}) = \frac{(x - x_k) + i(y - y_k)}{\sqrt{(x - x_k)^2 + (y - y_k)^2}} \psi_0(\mathbf{r}), \quad (6)$$

with $\sqrt{x_k^2 + y_k^2} < R_+$. Note that this state can be written as $\psi' = e^{i\varphi_k} \psi_0$, where φ_k is the azimuthal angle around the axis (x_k, y_k, z) , and hence, the operation we have performed on $\psi_0(\mathbf{r})$ represents a phase imprint to the original state. Therefore, while the density profiles of ψ_0 and ψ' are the same, the state ψ' has an imprinted velocity field $\mathbf{v} = (\hbar/m) \nabla \varphi_k$. This field is irrotational everywhere except at the vorticity line

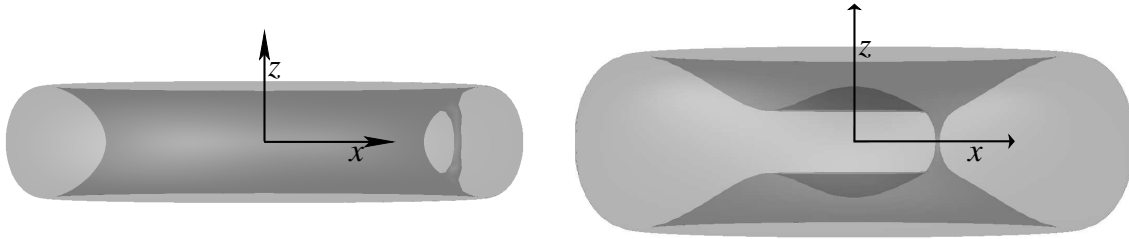


Figure 3. Three-dimensional views of the condensate containing different vortex states. In the left and right panels we depict surfaces of constant density $\rho a_{\text{ho}}^3 \simeq 150$ and 3, respectively. *Left panel:* a vortex with a bent vorticity line that crosses the $z = 0$ plane through the point $(14, 0, 0)$. *Right panel:* the stable straight vorticity line that crosses the $z = 0$ plane at the point $(6, 0, 0)$.

(x_k, y_k, z) . In general the vorticity line is defined as the set of points where

$$\boldsymbol{\omega}(\mathbf{r}) = \nabla \times \mathbf{v}(\mathbf{r}) \quad (7)$$

is nonzero. The important feature of this method is that the process of minimization may bend and move this curve, but does not destroy it. More general distributions of vorticity lines can be generated with an extended version of this method, but in this paper we restrict ourselves to the generation of a singly quantized vortex.

Using ψ' as the initial guess of the minimization, the program in a few iterations generates a density hole around the vorticity line, maintaining the original circulation.

In figure 3 we show surfaces of constant density for two vortex states which were obtained using this method. In the calculations of this particular figure we have changed the ω_z frequency to $\omega_z = \omega_r$, in order to better illustrate the shape of the vortices. In the left panel we show a vortex which was obtained after a few iterations from a vorticity line generated near $(14, 0, z)$. It may be seen that the method allows the vortex to bend in order to minimize the energy.

As the minimization proceeds the vortex moves towards an energy minimum and the state finally converges to the stable vortex, whose vorticity line is at $(6, 0, z)$. This final configuration is displayed in the right panel of figure 3.

In figure 4 we show the density profile of the stable vortex compared to that of the ground state. It may be seen that the vortex is located around the minimum of the ground-state density. Note that this method provides a vortex density shaped as if having used an effective centrifugal potential, that is, for instance, it vanishes at the core and its size is of the order of the healing length.

Note that the method of minimization we have adopted is subject to the constraint of wavefunction normalization only. In nonrotating condensates, a variety of numerical techniques, specially in two dimensional systems, have been applied to find distinct types of stationary vortices obtained from the GP functional with different constraints (see,

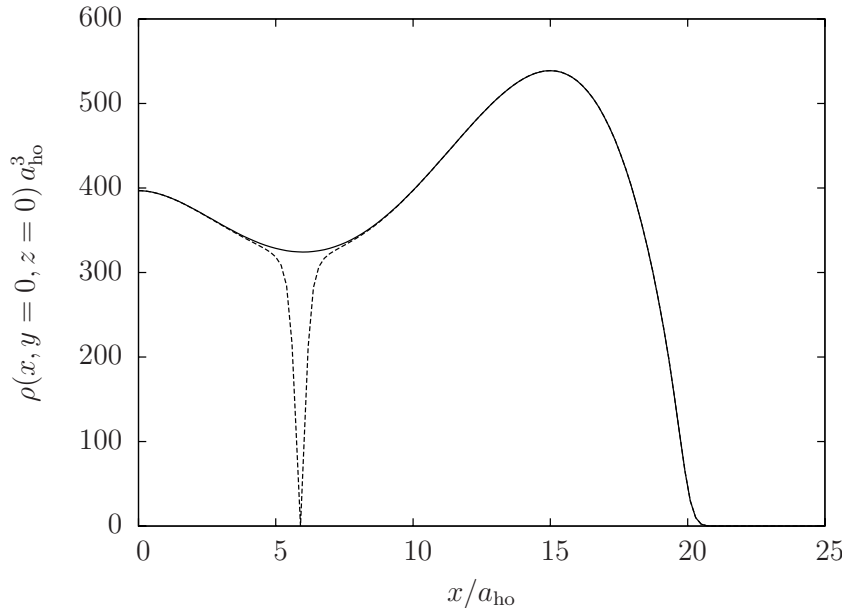


Figure 4. Density profiles of the ground state (solid line) and the stable vortex (dashed line) at $y = 0$ and $z = 0$.

e.g., [14–16, 26]). A single vortex may be also obtained by using the standard centrifugal potential (CP) term in the energy [24]. This method has a rapid convergence but the position of the stable vortex has to be specified in advance. An additional drawback of this method is that, in three dimensional systems the vortex line cannot bend.

4. Parametrization of the vortex kinetic energy

In this section we shall derive an approximate analytical expression for the kinetic energy E_v^K of a vortex shifted a distance r_0 from the z -axis.

As we have restricted our analysis to nearly pancake-shaped condensates, we can assume that the vortex is not bent. In other words we shall consider a straight vortex, parallel to the z -axis, and thus its velocity field does not depend on the z -coordinate.

The kinetic energy due to the vortex velocity field is

$$E_v^K = \frac{1}{2} m \int \int \int dx dy dz \rho_v(\mathbf{r}) v_{r_0}^2(x, y), \quad (8)$$

where $\rho_v(\mathbf{r})$ is the density of the condensate with a vortex.

In the limit of large N we may assume that the shape of ρ_v is almost the same as the ground-state, except for the presence of the core. In addition we consider that the most important contribution to the integral in (8) should stem from a narrow region around the core, still large compared to the healing length, and that the ground-state density varies smoothly in this region. Defining r_\perp as the radial coordinate measured from the vortex position r_0 , the energy may be written as

$$E_v^K = \frac{1}{2} m \int \int dr_\perp^2 dz \rho_0(r_0, z) f_{r_0}(r_\perp, z) v^2(r_\perp). \quad (9)$$

Note that at $r_\perp = 0$ the velocity diverges as $v(r_\perp) = \hbar/(mr_\perp)$. In (9) we have introduced the form factor $f_{r_0}(r_\perp, z) = \rho_v(r_\perp, z)/\rho_0(r_0, z)$ for describing the shape of the core. As we are considering a pancake-shaped condensate, we can evaluate the integral at $z = 0$. Then the energy reduces to

$$E_v^K = \frac{1}{2} m \ell \rho_0(r_0, 0) \int dr_\perp^2 f_{r_0}(r_\perp, 0) v^2(r_\perp), \quad (10)$$

where ℓ is the width of the condensate in the z -direction. Finally we shall assume that the structure of the vortex core does not change appreciably along the condensate i.e., $f_{r_0}(r_\perp, 0) = f(r_\perp, 0)$. In conclusion, under all the above assumptions we may approximate

$$E_v^K \sim \rho_0(r_0, 0) F. \quad (11)$$

This formulae is similar to, e.g. equation (51) of [18] derived for a strictly 2D system, with the difference that in that work the factor F takes an analytical form as a result of additional assumptions made on the condensate profile. In this work we will use the factor F as a single fitting parameter for reasons that will become clear in the following section.

5. Vortex energy: numerical calculations

We have computed the energy of a state with a single off-axis vortex E_v^s , using the formulae (1) by means of both the CP and the NPI methods. In each case we have employed the conjugate gradient technique with a spatial grid of $256 \times 256 \times 128$ points in the x, y, z directions, respectively. The minimizations were performed until a precision of 10^{-8} in the chemical potentials was achieved. In figure 5 we show the vortex energy defined as $E_v = E_v^s - E_0$, where E_0 is the ground-state energy.

The points along the NPI curve were obtained from three different runs starting from imprinted vorticities next to $r = 0$, and on the left and right of R_+ . Once the vortex core was generated, we evaluated the energy as a function of its position in the plane $z = 0$. Note that the run that starts on the right hand side of the top of the energy barrier, i.e. on the right of R_+ , moves towards outside the condensate. When the vortex is outside the condensate, its energy vanishes and the state coincides with the ground state.

The CP curve has been obtained by specializing the GP energy functional with a straight singly quantized vortex state fixed at (x_0, y_0, z) , i.e., by setting the full complex wavefunction to $\psi = e^{i\varphi_0} f(\mathbf{r}_\perp)$ and minimizing the energy respect to the real function $f(\mathbf{r}_\perp)$, as described in Ref. [24]. The phase factor gives rise to the effective centrifugal potential

$$V_C(\mathbf{r}) = \frac{\hbar^2}{2m} ((x - x_0)^2 + (y - y_0)^2)^{-1} \quad (12)$$

in the simplified GP equation for $f(\mathbf{r}_\perp)$.

We have also plotted the curve obtained from the expression (11) with the factor $F = 30$ fitted to the energy minimum at $r_0 = 6$. Note that in the present numerical

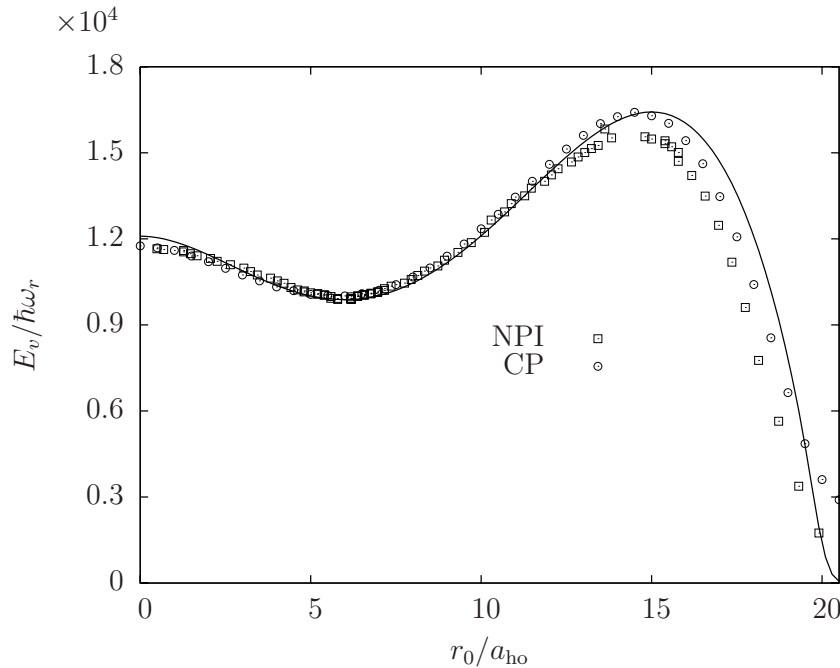


Figure 5. Vortex energy E_v as a function of the position of the core at the plane $z = 0$. The squares (circles) indicate NPI (CP) calculations and the curve obtained from the expression (11), with a factor $F = 30$, is depicted with a solid line.

calculation there exist another, not fully negligible, contributions to the energy E_v besides E_v^K . Nevertheless the curve is well reproduced by the estimate (11) using an appropriate value of F .

Near the maximum R_+ the NPI method provides a lower energy than the other approaches due to the possibility this method offers in bending vortices.

6. Summary and concluding remarks

We have introduced a static fourth-order polynomial trapping potential that can sustain locally stable off-axis vortices. We have also developed a numerical method for the generation of vortices without resorting to the addition of a centrifugal potential or the application of a rotating frame. On the other hand, we have computed the vortex energy as a function of its position using both the CP and the NPI methods, and find that a well defined energy barrier is obtained. We have also shown that this energy E_v can be approximated by a single fitting parameter times the ground-state density. This fitting parameter has been adjusted to the local energy minimum. Note that the profile of the barrier constitutes an essential ingredient when studying mechanisms of decay of metastable states. Therefore it is important to have efficient methods for its computation.

The scenario we have introduced may be useful, e.g., for numerically studying the dynamics of vortices in a spatially inhomogeneous superfluid [17–22]. In presence of many vortices, the dynamics of a particular vortex is dominated by the velocity fields of

the others, while in their absence its velocity is proportional to the gradient of the ground state density. With this trapping potential, a single vortex may precesses in two different directions depending at which side of the stationary positions it is located. Finally, this trapping potential may be also suitable for sustaining arrays of stable vortices, as for example, a ring of vortices with an arbitrary radius which can be modelled by changing the parameters r_1 and r_2 .

Acknowledgments

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