Structure and Stability of Vortices in Dilute Bose-Einstein Condensates at Ultralow Temperatures

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(Received 5 June 2000)

We compute the structure of a quantized vortex line in a harmonically trapped dilute atomic Bose-Einstein condensate using the Popov version of the Hartree-Fock-Bogoliubov mean-field theory. The vortex is shown to be (meta)stable in a nonrotating trap even in the zero-temperature limit, thus confirming that weak particle interactions induce for the condensed gas a fundamental property characterizing "classical" superfluids. We present the structure of the vortex at ultralow temperatures and discuss the crucial effect of the thermal gas component to its energetic stability.

DOI: 10.1103/PhysRevLett.86.2704 PACS numbers: 03.75.Fi, 05.30.Jp, 32.80.Pj, 67.40.Db

Dilute atomic Bose-Einstein condensates (BECs) have been the subject of numerous experimental and theoretical studies since the first landmark experiments in 1995 [1–3]. These quantum fluids are unique in providing an opportunity to investigate how the phenomenon of Bose-Einstein condensation is affected by weak particle interactions. The fundamental question, whether superfluidity can be sustained by particle interactions in such systems, has still remained partly open despite extensive research.

The existence of stable, dissipationless vortices is a feature characteristic to superfluid behavior. This aspect on the superfluid properties of dilute BECs is especially topical due to the recent experimental realizations of vortices in such systems [4,5]. The stability of vortex structures has been under vigorous theoretical analysis [6–18]. It has been shown that vortices in cylindrically trapped condensates are unstable within the Bogoliubov mean-field approximation [8–10,16,19] unless the system is continuously driven by a suitable rotating perturbation [10,12,15]. On the other hand, by taking into account effects of the thermal gas component in the system, vortices have been shown to become (meta)stable at high enough temperatures even in a nonrotating trap, or when a suitable external pinning potential is applied [13].

The absence of dissipation in the superfluid flow implies that a circulating current persists even when the system is not rotated by an external perturbation. "Classical" superfluid behavior thus implies stability of vortices even in a nonrotating vessel. Strictly speaking, such states are local minima of free energy and only metastable, the global minimum naturally corresponding to a nonrotating state. However, in order to investigate the superfluid properties of dilute boson condensates, it is just this kind of local energetic stability of vortices that needs to be clarified.

In this Letter we present results of computations concerning the structure of a cylindrically trapped dilute BEC containing a vortex line and show that such states are locally energetically stable at all temperatures $T < T_c$ (T_c denotes the critical temperature of condensation) even in a nonrotating trap without additional pinning potentials. In this respect such systems are indeed shown to behave like classical superfluids. We also discuss the obvious discrepancy between this result and the predictions of the Bogoliubov approximation, and the role of the thermal gas fraction in stabilizing the vortex state in the zero-temperature limit.

We consider a dilute Bose-condensed gas consisting of atoms with mass m, trapped by a radial harmonic potential $V_{\rm trap}(\mathbf{r}) = \frac{1}{2} m\omega_r^2 r^2$ in cylindrical coordinates $\mathbf{r} = (r, \theta, z)$. The particle interactions are modeled by an effective low-temperature contact potential $V_{\rm int}(\mathbf{r}, \mathbf{r}') = g\delta(\mathbf{r} - \mathbf{r}')$, with the bare interaction constant g and s-wave scattering length for binary collisions a related by $g = 4\pi\hbar^2 a/m$. Assuming the total particle number in the condensate to be large enough to justify grand canonical formalism, the equilibrium condensate wave function $\phi(\mathbf{r})$ satisfies the generalized Gross-Pitaevskii (GP) equation [20]

$$\{\mathcal{H}_0 + U_c(\mathbf{r})|\phi(\mathbf{r})|^2 + 2U_e(\mathbf{r})\rho(\mathbf{r})\}\phi(\mathbf{r}) = \mu\phi(\mathbf{r}), \tag{1}$$

where $\mathcal{H}_0 = -\hbar^2\nabla^2/2m + V_{\rm trap}(\mathbf{r})$ is the bare single-particle Hamiltonian for the trap, μ is the chemical potential, and $\rho(\mathbf{r})$ is the density of the noncondensed gas. Functions $U_c(\mathbf{r})$, $U_e(\mathbf{r})$ are effective interaction couplings for various mean-field approximations—for the Popov version they are simply chosen as $U_c(\mathbf{r}) = U_e(\mathbf{r}) \equiv g$. In addition, we have performed computations within so-called G1 and G2 approximations, which are gapless mean-field theories taking into account effects of the background gas on colliding atoms, neglected in the Popov approximation [21,22]. In the G1 version $U_e(\mathbf{r}) \equiv g$ and $U_c(\mathbf{r}) = g[1 + \Delta(\mathbf{r})/\phi^2(\mathbf{r})]$, where $\Delta(\mathbf{r})$ is the anomalous average of two Bose field operators; for G2 one chooses $U_e(\mathbf{r}) = U_c(\mathbf{r}) = g[1 + \Delta(\mathbf{r})/\phi^2(\mathbf{r})]$. The usual procedure of diagonalizing the mean-field Hamiltonian by a Bogoliubov transformation yields coupled eigenvalue equations for the bosonic quasiparticle

 0031-9007/01/86(13)/2704(4)$15.00

amplitudes $u_q(\mathbf{r})$, $v_q(\mathbf{r})$, and the eigenenergies E_q of the form [20]

$$\mathcal{L}\, u_q(\mathbf{r}) + U_c(\mathbf{r})\phi^2(\mathbf{r})v_q(\mathbf{r}) = E_q u_q(\mathbf{r}), \tag{2a}$$

$$\mathcal{L}\, v_q(\mathbf{r}) + U_c(\mathbf{r})\phi^{*2}(\mathbf{r})u_q(\mathbf{r}) = -E_q v_q(\mathbf{r}). \tag{2b}$$

Above, $\mathcal{L} \equiv \mathcal{H}_0 - \mu + 2U_c(\mathbf{r})|\phi(\mathbf{r})|^2 + 2U_e(\mathbf{r})\rho(\mathbf{r})$ and q denotes quantum numbers specifying the quasiparticle states. In addition, we have self-consistency relations for the noncondensate density $\rho(\mathbf{r})$ and for the anomalous average $\Delta(\mathbf{r})$:

$$\rho(\mathbf{r}) = \sum_q [(|u_q(\mathbf{r})|^2 + |v_q(\mathbf{r})|^2)n(E_q) + |v_q(\mathbf{r})|^2], \tag{3}$$

$$\Delta(\mathbf{r}) = \sum_q [2u_q(\mathbf{r})v_q^*(\mathbf{r})n(E_q) + u_q(\mathbf{r})v_q^*(\mathbf{r})], \tag{4}$$

where $n(E_q) = (e^{E_q/k_B T} - 1)^{-1}$ is the Bose distribution function. The anomalous average is ultraviolet divergent, and we renormalize it by subtracting the last term in the sum of Eq. (4) [23].

Considering a condensate penetrated by a single vortex line, we search for solutions of the form $\phi(\mathbf{r}) = \phi(r)e^{im\theta}$, where m denotes the number of circulation quanta of the vortex. In this Letter we restrict ourselves to the case $m = 1$ due to the instability of multiquantum vortices [14,16,18]. By utilizing the cylindrical symmetry, Eqs. (1) and (2) can be reduced to radial equations, which we discretize using a finite-difference method. Dirichlet boundary conditions are imposed at $r = R$, the radius R chosen large enough for finite-size effects for the structure of the vortex to be negligible. In the z direction we impose periodic boundary conditions at $z = \pm L/2$, thus modeling a system in the limit of a very weak axial trapping potential. Because of cylindrical symmetry, the quasiparticle amplitudes can be chosen to be of the form

$$u_q(\mathbf{r}) = u_q(r)e^{iq_z(2\pi/L)z + i(q_\theta + m)\theta}, \tag{5a}$$

$$v_q(\mathbf{r}) = v_q(r)e^{iq_z(2\pi/L)z + i(q_\theta - m)\theta}, \tag{5b}$$

where q_θ and q_z are integer angular and axial momentum quantum numbers, respectively. Discretization transforms Eqs. (2) to a narrow-banded matrix eigenvalue problem, which we solve using the Lanczos algorithm implemented in the ARPACK subroutine libraries [24,25]. The nonlinear Gross-Pitaevskii equation is solved using finite-difference discretization and an overrelaxation method. For a given value of the chemical potential μ, the solution of the GP equation and the noncondensate density are integrated to find out the total particle number, and the process is iterated until the chemical potential corresponds to the preset total number of particles. The solution of the GP equation can be mapped to a zero-energy solution of Eqs. (2), thus providing a test for the accuracy and consistency of the numerical methods used to solve these equations. We search self-consistent solutions for Eqs. (1)–(4) using an iterative scheme: The condensate wave function and the chemical potential corresponding to a preassigned total number of particles are computed by solving the GP equation. Using the quasiparticle states obtained from Eqs. (2), new mean-field potentials are computed using the self-consistency equations. The whole procedure is repeated until convergence to a desired accuracy. In order to stabilize the iteration at low temperatures, we use underrelaxation in updating the mean-field potentials.

The physical parameter values for the gas and the trap were chosen to be the same as in Ref. [13]. The gas consists of sodium atoms with mass $m = 3.81 \times 10^{-26}$ kg and s-wave scattering length $a = 2.75$ nm. The frequency of the trap is $\nu_r = \omega_r/2\pi = 200$ Hz, and the density of the system is determined by treating $N = 2 \times 10^5$ atoms in the computational domain with dimensions $R = 20\ \mu$m and $L = 10\ \mu$m. The critical condensation temperature for the system is approximately $T_c \approx 1\ \mu$K. The spatial grid for discretizing the quasiparticle eigenequations was chosen dense enough to guarantee a relative accuracy of 10^{-3} for the energy of the lowest excitation, and better than 10^{-4} for the other states.

Results of the self-consistent computations performed within the Popov approximation are shown in Figs. 1–4. Figure 1 displays part of the self-consistent quasiparticle excitation spectrum for the condensate vortex state at the temperature $T = 100$ nK. Only states with $q_z = 0, 1$, which contain the excitations of lowest energy, are shown. These states determine the local energetic stability of the vortex configuration: If there exists a quasiparticle excitation with negative energy, the condensate can lower

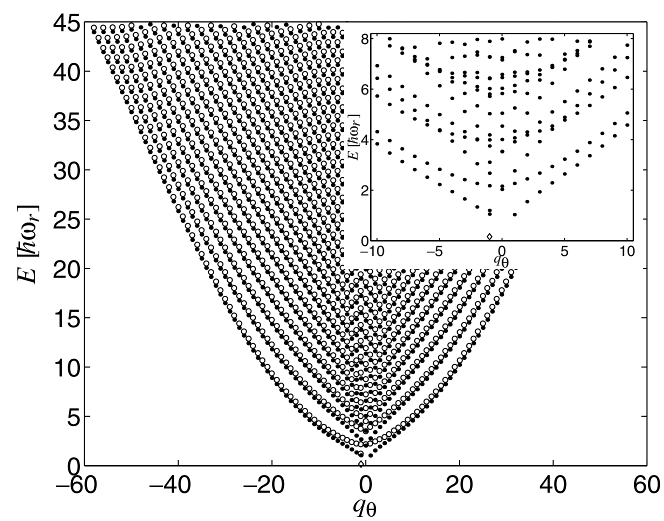

FIG. 1. Part of the self-consistent quasiparticle excitation spectrum at temperature $T = 100$ nK for the harmonically trapped condensate containing a single-quantum vortex line. Only states with axial momentum quantum numbers $q_z = 0$ (dots) and $q_z = 1$ (circles) are shown. The lowest Kelvin mode state, the LCLS, is denoted by a diamond. The inset presents a blowup of the lowest part of the full spectrum.

its energy by exciting this negative bosonic mode, the state thus being prone to collapse. For single-quantum vortices the lowest excitations with $q_\theta = -1$, the so-called Kelvin mode states, form standing waves localized at the vortex core, the energies of these states being substantially lower than those for other angular momentum quantum numbers. The sign of the energy of the lowest Kelvin mode excitation, the lowest core localized state (LCLS), determines the local energetic stability of the vortex. The LCLS is denoted by a diamond in Fig. 1. Because of the very low energy of the LCLS compared to the other excitations, its contribution to the mean-field potentials in the core region becomes dominant in the zero-temperature limit. On the other hand, even minor changes in the potential functions affect the energy of the LCLS, thus altering its contribution drastically via the sensitive Bose factor. This behavior makes the iteration process extremely delicate at low temperatures [13], requiring the use of suitable underrelaxation methods.

The temperature dependence of the excitation energy of the LCLS is shown in Fig. 2. By carefully adjusting underrelaxation in the iteration procedure, we are able to compute the self-consistent structure of the vortex down to the temperature of $T = 1$ nK. The convergence at these temperatures is slow, but unquestioned. Especially, it was confirmed that the iteration converges to the same solution irrespective of the initial ansatz used. However, it seems obvious that with additional computational effort one could reach even lower temperatures. The result shows that although the energy of the LCLS approaches zero in the low-temperature limit, as expected, the vortex configuration is locally stable at all temperatures $T < T_c$ [13]. We obtained the same result also using the G1 and G2 approximations.

The local energetic stability of the vortex within the Popov, G1, and G2 [26] approximations is to be compared with the instability predicted by the Bogoliubov approximation [9], which does not treat the thermal part of the gas self-consistently. Figure 3 shows the density profiles of the condensate and the noncondensate at ultralow temperatures. The thermal gas is concentrated in the vortex core, where it fills the space left by the condensate and exerts an outward pressure on it, preventing the condensate from collapsing into the core. Self-consistent treatment of the thermal gas fraction is thus crucial in determining the stability of vortices in such systems, as seen in the discrepancy between the predictions of the Popov, the G1 and the G2, and, on the other hand, the Bogoliubov approximation. At temperatures of the order of T_c, the validity of the Bogoliubov approximation is expected to be questionable due to the substantial thermal gas fraction. It is to be noted that it can fail also in the low-temperature limit in certain respects, the stability of the vortex state being one example. This is due to the nonvanishing, residual noncondensate fraction present in interacting systems even in the zero-temperature limit. Figure 4 displays the computed thermal gas fraction at ultralow temperatures. It clearly shows the residual thermal fraction, which stabilizes the vortex at ultralow temperatures.

It is to be noted that the positivity of the LCLS energy implies that vortices slightly displaced from the symmetry axis of the trap precess in the direction opposite to the condensate flow around the core [27]. Recent experiments, however, show precession in the direction of the flow, except for a minority of the so-called rogue vortices [28]. This seems to imply a negative LCLS energy, in agreement with the zero-temperature Bogoliubov approximation. The apparent discrepancy between the experiments and the predictions of the self-consistent approximations could be due to insufficient thermalization in the experiments of the gas in the region of the (moving) vortex core. We expect that investigation of the validity of this assumption will

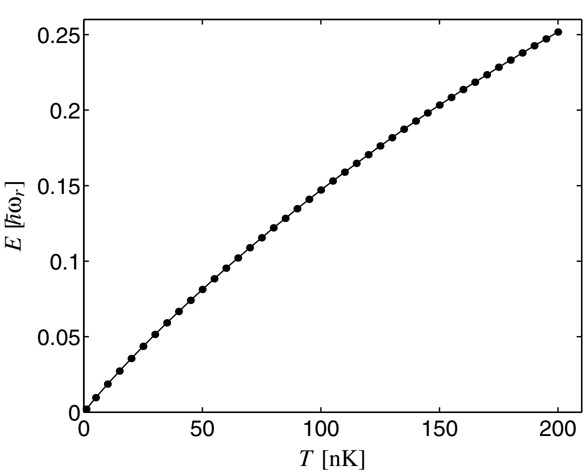

FIG. 2. Energy of the lowest excitation, the LCLS, at temperatures $T = 1-200$ nK ($T_c \approx 1$ μK). The finite positive value of the lowest excitation frequency implies the vortex to be locally energetically stable.

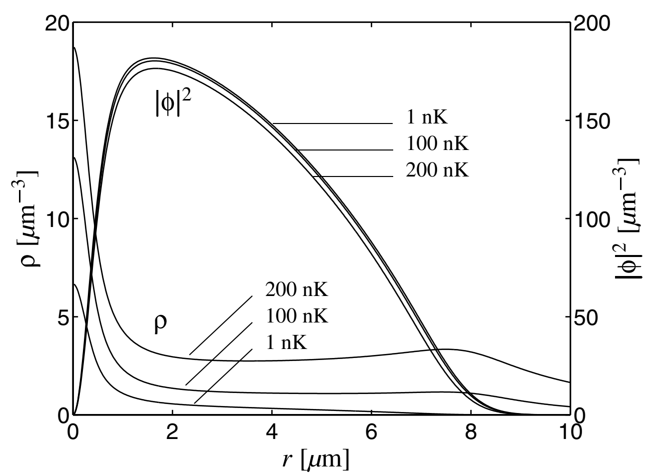

FIG. 3. Condensate and thermal gas density profiles at temperatures $T = 1$, 100, and 200 nK. The noncondensate fills the space left by the condensate in the vortex core, thus exerting an outward pressure which stabilizes the vortex configuration.

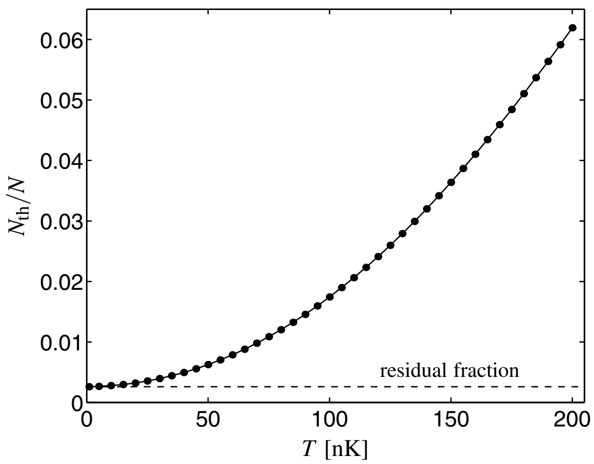

FIG. 4. Noncondensate fraction as a function of temperature for the vortex configuration. Because of particle interactions, there exists a residual thermal gas fraction even in the zero-temperature limit.

further clarify the role of quasiparticles in stabilizing vortices in weakly interacting Bose-Einstein condensates.

In conclusion, we have computed within self-consistent mean-field theories the structure of a cylindrically trapped, dilute atomic Bose-Einstein condensate penetrated by a vortex line. The vortex state is shown to be locally energetically stable in a nonrotating system even in the zero-temperature limit, thus confirming the system to act in this respect like a superfluid. The thermal gas concentrated in the vortex core is shown to have a crucial effect in stabilizing the vortex state even at ultralow temperatures, due to a residual noncondensate fraction present in interacting systems in the zero-temperature limit.

We thank the Center for Scientific Computing for computer resources. The Academy of Finland and the Graduate School in Technical Physics are acknowledged for support.

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