Adiabaticity Criterion for Moving Vortices in Dilute Bose-Einstein Condensates

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(Received 18 May 2001; published 15 November 2001)

Considering a moving vortex line in a dilute atomic Bose-Einstein condensate within time-dependent Hartree-Fock-Bogoliubov-Popov theory, we derive a criterion for the quasiparticle excitations to follow the vortex core rigidly. The assumption of adiabaticity, which is crucial for the validity of the stationary self-consistent theories in describing such time-dependent phenomena, is shown to imply a stringent criterion for the velocity of the vortex line. Furthermore, this condition is shown to be violated in the recent vortex precession experiments.

DOI: 10.1103/PhysRevLett.87.230403 PACS numbers: 03.75.Fi, 05.30.Jp, 67.40.Db

Since the first experimental realizations of Bose-Einstein condensation in dilute, harmonically trapped atomic gases [1], there has been great interest to investigate the superfluid properties of these unique quantum systems. Because of the inherent connections between quantized vorticity and superfluidity, this interest culminated as the creation of vortices in trapped condensates was demonstrated [2]. The recent experimental advances in manipulating vortices and observing their dynamics are providing efficient tools to study the physics of these interacting many-particle systems and to relate it to the quantitative predictions of thermal field theories.

The structure and, in particular, the stability of vortices in dilute Bose-Einstein condensates (BECs) has been under an extensive theoretical analysis [3]. The majority of the studies have been carried out within the zero-temperature mean-field formalism consisting of the Gross-Pitaevskii (GP) and Bogoliubov equations. Within the Bogoliubov approximation (BA), the excitation spectra of vortex states in statically trapped condensates have been shown to contain at least one mode with positive norm but negative energy [4]. These anomalous modes have crucial consequences for the superfluid properties of the condensates, since they imply the vortices to be energetically unstable in nonrotating traps. Furthermore, these states have been shown to manifest themselves in the precession of the vortex line about the symmetry axis of the trap, with the precession frequency and direction determined by the excitation energy—especially, the negative energies imply precession in the direction of the condensate flow [5].

The predictions of the Bogoliubov approximation agree well with the experiments. The critical trap rotation frequencies for vortex nucleation can be understood theoretically to good accuracy [6]. Also, the precession of vortices predicted by the GP equation has been experimentally observed [7]. The precession frequency and, in particular, its direction are in line with expectations based on the BA. In general, the mean-field theory has turned out to be remarkably successful in describing trapped BECs, including the vortex states and their dynamics [8].

However, the situation changes when the analysis is taken beyond the zero-temperature BA by self-consistently including the effects of the thermal gas component. Stationary self-consistent solutions for vortex states within the Popov approximation (PA) and its recently proposed extensions contain no anomalous modes even in the zero-temperature limit [9,10]. This is due to the partial filling of the vortex core with the noncondensate, which serves to lift the anomalous quasiparticle states to positive energies. The positive precession mode energies, in turn, imply vortex precession opposite to the condensate flow, in evident contradiction with the experimental observations and the predictions of the BA. In light of the success of the self-consistent approximations in predicting excitation spectra for irrotational condensates [11,12], this discrepancy is surprising. In addition, the close agreement of the BA with the results of the vortex precession experiments implies that the mean-field approximation itself is not the cause of the failure of the PA.

We suggest that the apparent disagreement between the PA and the experiments could be due to incomplete thermalization and/or inadequacy of the quasistatic formalism in describing moving vortices. In order to clarify the latter possibility, we show in this Letter that the validity of the quasistatic self-consistent mean-field treatment in modeling moving vortices imposes for the vortex velocity a stringent criterion, which seems to be violated in the precession observations reported thus far. This implies that at the observed velocities the quasiparticles cannot follow the vortex core rigidly, and its structure and spectrum are deformed from those of a static vortex.

In order to describe the dynamics of trapped BECs, we use a time-dependent mean-field formalism based on the Popov approximation [13]. Working in the grand-canonical formalism, we start with the Heisenberg equation of motion,

$$i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r},t) = \mathcal{H}_0(\mathbf{r})\psi(\mathbf{r},t) + g\psi^\dagger(\mathbf{r},t)\psi(\mathbf{r},t)\psi(\mathbf{r},t), \tag{1}$$

for the field operator $\psi(\mathbf{r},t)$ of a dilute boson gas. Above, $\mathcal{H}_0(\mathbf{r}) \equiv -\hbar^2\nabla^2/2m + V_{\mathrm{tr}}(\mathbf{r}) - \mu$ is the grand-canonical one-particle Hamiltonian corresponding to the trapping potential $V_{\mathrm{tr}}(\mathbf{r})$ and the chemical potential μ, and the coupling constant g is related to the s-wave scattering length a by $g = 4\pi\hbar^2 a/m$. Inserting into the nonequilibrium average of Eq. (1) the Bogoliubov decomposition

$$\psi(\mathbf{r},t) = \Phi(\mathbf{r},t) + \tilde{\psi}(\mathbf{r},t) \tag{2}$$

of the field operator in terms of the c-number condensate wave function $\Phi(\mathbf{r},t) = \langle\psi(\mathbf{r},t)\rangle$ and the noncondensate field operator $\tilde{\psi}(\mathbf{r},t)$, and treating the expectation values of the noncondensate operator products according to the Popov mean-field scheme, we arrive at the generalized GP equation,

$$i\hbar\frac{\partial}{\partial t}\Phi(\mathbf{r},t) = \mathcal{L}(\mathbf{r},t)\Phi(\mathbf{r},t) - gn_c(\mathbf{r},t)\Phi(\mathbf{r},t), \tag{3}$$

for the condensate wave function. Above, $\mathcal{L}(\mathbf{r},t) \equiv \mathcal{H}_0(\mathbf{r}) + 2gn(\mathbf{r},t)$, and

$$n_c(\mathbf{r},t) = |\Phi(\mathbf{r},t)|^2, \tag{4a}$$

$$\tilde{n}(\mathbf{r},t) = \langle\tilde{\psi}^\dagger(\mathbf{r},t)\tilde{\psi}(\mathbf{r},t)\rangle, \tag{4b}$$

$$n(\mathbf{r},t) = n_c(\mathbf{r},t) + \tilde{n}(\mathbf{r},t) \tag{4c}$$

denote the condensate, noncondensate, and total densities, respectively. Correspondingly, within the Popov mean-field approximation, one finds

$$i\hbar\frac{\partial}{\partial t}\tilde{\psi}(\mathbf{r},t) = \mathcal{L}(\mathbf{r},t)\tilde{\psi}(\mathbf{r},t) + g\Phi^2(\mathbf{r},t)\tilde{\psi}^\dagger(\mathbf{r},t), \tag{5}$$

for the equation of motion of the noncondensate field operator. Substituting into Eq. (5) the Bogoliubov transformation

$$\tilde{\psi}(\mathbf{r},t) = \sum_n[u_n(\mathbf{r},t)\alpha_n - v_n^*(\mathbf{r},t)\alpha_n^\dagger] \tag{6}$$

of the field operator in terms of the bosonic quasiparticle operators α_n and $\alpha_n^\dagger$, we find that the quasiparticle amplitudes $u_n(\mathbf{r},t)$ and $v_n(\mathbf{r},t)$ satisfy the time-dependent Hartree-Fock-Bogoliubov-Popov (TDHFBP) equations:

$$i\hbar\frac{\partial}{\partial t}u_n(\mathbf{r},t) = \mathcal{L}(\mathbf{r},t)u_n(\mathbf{r},t) - g\Phi^2(\mathbf{r},t)v_n(\mathbf{r},t), \tag{7a}$$

$$-i\hbar\frac{\partial}{\partial t}v_n(\mathbf{r},t) = \mathcal{L}(\mathbf{r},t)v_n(\mathbf{r},t) - g\Phi^{*2}(\mathbf{r},t)u_n(\mathbf{r},t). \tag{7b}$$

Introducing the matrix notations,

$$f_n = \begin{pmatrix} u_n \\ v_n \end{pmatrix}, \qquad \mathcal{O} = \begin{pmatrix} \mathcal{L} & -g\Phi^2 \\ g\Phi^{*2} & -\mathcal{L} \end{pmatrix}, \tag{8}$$

the quasiparticle equations can be expressed in the compact form,

$$i\hbar\frac{\partial}{\partial t}f_n(\mathbf{r},t) = \mathcal{O}(\mathbf{r},t)f_n(\mathbf{r},t). \tag{9}$$

Here and henceforth, we suppress the arguments of functions when they are not needed for clarity. For convenience, we also define positive- and negative-sign scalar products of quasiparticle states by setting

$$\langle f_i|f_j\rangle_\pm \equiv \int d\mathbf{r}[u_i^*(\mathbf{r})u_j(\mathbf{r}) \pm v_i^*(\mathbf{r})v_j(\mathbf{r})]. \tag{10}$$

The requirement that the quasiparticle operators α_n, $\alpha_n^\dagger$ satisfy canonical bosonic commutation relations implies for the quasiparticle states the normalization $\langle f_i|f_j\rangle_- = \delta_{ij}$; correspondingly, only states with positive norm are to be included in the Bogoliubov transformation of Eq. (6). This normalization can be straightforwardly verified to be consistent with the TDHFBP equations.

In case the mean fields and, hence, the operator $\mathcal{O}(\mathbf{r},t)$ vary slowly in time, we expect that the solutions of the TDHFBP equations may be approximated by solving at each instant of time the corresponding quasistationary eigenequations:

$$E_n(t)f_n^{(0)}(\mathbf{r},t) = \mathcal{O}(\mathbf{r},t)f_n^{(0)}(\mathbf{r},t). \tag{11}$$

This adiabatic approximation is accurate if the transition rates, as determined by the exact time development, of the quasistationary states to each other are negligible. In order to formulate this criterion quantitatively, we follow the treatment of Ref. [14]. Let $\{f_i^{(0)}\}$ be a complete set of solutions of Eq. (11); especially, it contains the zero-energy solution $f_0^{(0)} \propto (\Phi_0, \Phi_0^*)^T$, where Φ_0 is the solution of the stationary GP equation. We orthonormalize the solutions by requiring

$$|\langle f_i^{(0)}|f_j^{(0)}\rangle_-| = \delta_{ij} \qquad (i \neq 0); \qquad \langle f_0^{(0)}|f_0^{(0)}\rangle_+ = 1. \tag{12a}$$

In addition, we may impose the condition [15]

$$\langle f_0^{(0)}|f_i^{(0)}\rangle_+ = 0 \qquad (i \neq 0). \tag{12b}$$

In order to analyze the transitions of the quasistationary states to each other, we expand the solutions of the TDHFBP equation in terms of them. Substitution of the ansatz

$$f_n(\mathbf{r},t) = \sum_j a_{nj}(t)f_j^{(0)}(\mathbf{r},t)e^{-(i/\hbar)\int_0^t E_j(t')dt'} \tag{13}$$

into Eq. (9) yields the coupled differential equations,

$$\sum_j[\dot{a}_{nj}f_j^{(0)} + a_{nj}\dot{f}_j^{(0)}]e^{-(i/\hbar)\int_0^t E_j(t')dt'} = 0, \tag{14}$$

where the dots above symbols denote time derivatives. Taking the positive scalar products of these equations with the state $f_0^{(0)}$, utilizing the orthonormalization relations (12), and solving for $\dot{a}_{n0}$, we find

$$\dot{a}_{n0} = -\sum_j a_{nj}e^{-(i/\hbar)\int_0^t E_j(t')dt'}\langle f_0^{(0)}|\dot{f}_j^{(0)}\rangle_+. \tag{15a}$$

In a similar manner, we derive the equations

$$\dot{a}_{nk} = -\sum_j a_{nj}e^{-(i/\hbar)\int_0^t[E_j(t')-E_k(t')]dt'}\langle f_k^{(0)}|\dot{f}_j^{(0)}\rangle_- \tag{15b}$$

for the coefficients with $k \neq 0$.

In order to estimate the decay of a state $f_n^{(0)}$, we assume that at time $t = 0$ its expansion coefficients are $a_{nj}(0) = \delta_{nj}$. Approximating the slowly varying scalar products and energy eigenvalues to be constant in time, and the decay to be negligible, such that we may also treat the a_{nj} coefficients on the right-hand sides (rhs) of Eqs. (15) as constants, we can integrate them to yield

$$a_{nk}(t) \simeq -\frac{i}{\omega_{nk}}(e^{-i\omega_{nk}t} - 1)\langle f_k^{(0)}|\dot{f}_n^{(0)}\rangle_\pm \,. \qquad (16)$$

Above, the positive scalar product is chosen for $k = 0$, the negative otherwise, and we have denoted $\omega_{nk} = (E_n - E_k)/\hbar$. Since the quasistationary states are orthonormalized, the requirement of negligible decay thus implies

$$\left| \frac{1}{\omega_{nk}}\langle f_k^{(0)}|\dot{f}_n^{(0)}\rangle_\pm \right| \ll 1 \,. \qquad (17)$$

Essentially, this is the validity criterion of the adiabatic approximation for the TDHFBP equations of a dilute boson gas.

Consider now the case of a vortex line precessing with frequency $\nu_{\rm pr}$ about a circular orbit of radius $R_{\rm pr}$ in a harmonically trapped condensate; for simplicity, we assume a trapping potential of the form $V_{\rm tr} = \frac{1}{2}m\omega_r^2 r^2$ in cylindrical coordinates $\mathbf{r} = (r, \theta, z)$, and the vortex line to be directed along the z axis [16]. In view of the differences in the vortex-core structure between the BA and the self-consistent approximations, it is especially interesting to find out whether the lowest-energy quasiparticles, which constitute the major contribution to the noncondensate filling the vortex core, can follow the moving vortex line rigidly, i.e., adiabatically. In order to assess the validity of the criterion (17) for such states, we use the estimate

$$\langle f_k^{(0)}|\dot{f}_n^{(0)}\rangle_\pm \simeq \mathbf{v}\cdot\langle f_k^{(0)}|\nabla f_n^{(0)}\rangle_\pm \,, \qquad (18)$$

where $\mathbf{v}$ is the velocity of the vortex line. This approximation treats accurately the region in the vicinity of the vortex line, although it is exact only for a uniform vortex motion. Furthermore, supposing the precession orbit is not too near the condensate boundary, we may use the quasiparticle states of a system with a vortex located in the center of the trap to estimate the scalar products on the rhs of Eq. (18). Such a system is cylindrically symmetric, and the quasiparticle eigenstates can be chosen to be of the form

$$u_q(\mathbf{r}) = \mathrm{u}_q(r)e^{iq_z(2\pi/L)z + i(q_\theta+1)\theta} \,, \qquad (19a)$$

$$v_q(\mathbf{r}) = \mathrm{v}_q(r)e^{iq_z(2\pi/L)z + i(q_\theta-1)\theta} \,, \qquad (19b)$$

where q_θ and q_z are integer angular and axial momentum quantum numbers, respectively, and q denotes the complete set of quantum numbers for the states. Calculation of the required matrix elements is straightforward for these states—the result is

$$\begin{aligned} vI_{qq'} &\equiv \mathbf{v}\cdot\langle f_q^{(0)}|\nabla f_{q'}^{(0)}\rangle_\pm \\ &\simeq -\frac{v}{2}\delta_{q_z q_z'}\delta_{|q_\theta - q_\theta'|,1}\int_0^\infty dr\left[r\left(\mathrm{u}_q^*\frac{d\mathrm{u}_{q'}}{dr} \pm \mathrm{v}_q^*\frac{d\mathrm{v}_{q'}}{dr}\right) + (q_\theta' - q_\theta)[(q_\theta'+1)\mathrm{u}_q^*\mathrm{u}_{q'} \pm (q_\theta'-1)\mathrm{v}_q^*\mathrm{v}_{q'}]\right], \end{aligned} \qquad (20)$$

where $v = |\mathbf{v}|$ is the magnitude of the velocity of the vortex line, and the states are normalized according to $\int_0^\infty r\,dr(|u_q|^2 \pm |v_q|^2) = 1$, with the plus (minus) sign used for the zero-energy condensate state (other states). Equations (17), (18), and (20) finally yield the criterion,

$$v \ll v_{qq'} \equiv \left|\frac{\omega_{qq'}}{I_{qq'}}\right| \qquad \text{(for all } q\text{)}\,, \qquad (21)$$

for the velocity of the precessing vortex in order for the state $f_{q'}^{(0)}$ to follow the vortex rigidly.

We have numerically computed adiabaticity velocities $v_{qq'}$ for a cylindrical condensate. The static HFB equations were solved self-consistently within the PA and its so-called $G1$ and $G2$ variants [12,17], in order to find the quasiparticle amplitudes $u_q(\mathbf{r})$, $v_q(\mathbf{r})$, and the respective eigenenergies—for details of the methods used in the computations, see Ref. [10]. In order to facilitate comparison with the vortex precession observations, we use parameter values which essentially correspond to the experiments reported in Ref. [7]. Especially, the radial trapping frequency was set to $\nu_r = \omega_r/2\pi = 7.8$ Hz, and the density of the trapped ^{87}Rb atoms was adjusted to yield a healing length $\xi = (8\pi n_0 a)^{-1/2} \approx 0.7\ \mu$m at temperature $T \approx 0.8T_{\rm BEC}$. Here n_0 denotes the peak density of the condensate, and the condensation temperature $T_{\rm BEC} \approx 30$ nK.

In the experiments, the observed precession radii were of the order of $R_{\rm pr} \simeq R/3 \simeq 10\ \mu$m, where R denotes the radius of the condensate [7]. Bare-core vortices were observed to precess in the direction of the condensate flow with frequency $\nu_{\rm pr} \approx 1.8$ Hz, which corresponds to a velocity $v_{\rm exp} = 2\pi R_{\rm pr}\nu_{\rm pr} \approx 0.1$ mm/s. This is to be compared with the computed velocities $v_{qq'}$ for the lowest quasiparticle states with $q_z = 0$, displayed in Fig. 1. Although $v_{\rm exp} \lesssim v_{qq'}$, we find the adiabaticity condition (21) not to be fulfilled. This suggests that, due to the deformation of the quasiparticle states, the noncondensate cannot follow the vortex line rigidly at these velocities. Especially interesting is the smallest adiabaticity velocity given by the decay of the so-called lowest core localized state (LCLS), which is the lowest excitation with $(q_\theta, q_z) = (-1, 0)$, and itself corresponds to the precession of the vortex. The LCLS has a crucial role in the filling of the vortex core with noncondensate, which stabilizes the static vortex state [9,10]. In fact, this state is almost solely responsible for the differences in the vortex structure between the BA and the PA in the low-temperature limit. Deformation of the LCLS

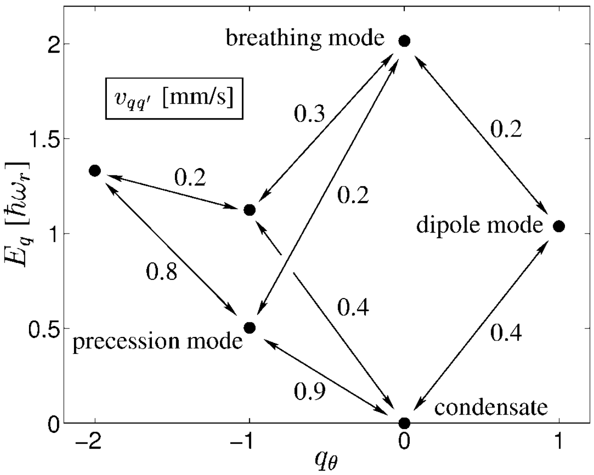

FIG. 1. Adiabaticity velocities determined by decay rates between the lowest vortex state excitations (dots) with $q_z = 0$. The data correspond to the PA and system temperature $T \approx 0.8T_{\rm BEC}$. The arrows denote the decay channels of the modes to each other, and the numbers the corresponding adiabaticity velocities $v_{qq'}$ [mm/s] [see Eq. (21)]. Note especially the low adiabaticity velocity given by the transitions between the precession and breathing modes—transitions from the precession mode are crucial in determining the deformation of the core structure of a moving vortex. Furthermore, due to weaker mutual couplings, the adiabaticity velocities given by transitions between states with higher energy or $q_z \neq 0$ were, in general, found to be larger. The degree of adiabaticity of a moving vortex is thus essentially determined by the lowest collective modes.

due to the vortex motion thus implies crucial modifications for the vortex core structure. The quasistationary noncondensate profile with a pronounced peak in the vortex core [10] is expected to be deformed to a smoother, more elongated profile because of the tendency of the quasiparticles to lag the vortex motion. Eventually, for high velocities the vortex tends to shake off the thermal cloud excess in the core, and one may argue that, in the limit of extreme nonadiabaticity, the BA would thus be more suitable in describing the vortex state than the quasistationary PA.

The given adiabaticity velocities also hold for the $G1$ and $G2$, since differences between the approximations turn out to be negligible in this respect. Computations with various parameter values also confirmed the validity of the criterion (21) to be largely independent of the specific values of the trapping frequency, the density of the gas, or the effective interaction between the atoms. Essentially, the adiabaticity of the system is determined by the precession radius $R_{\rm pr}$, via its proportionality to the velocity of the precessing vortex line. However, it seems that for currently realizable condensates the precession radii should be of the order of the vortex core radius or less for the adiabaticity criterion to be satisfied.

In conclusion, we have derived a criterion for the validity of the quasistationary approximation for a time-dependent mean-field formalism describing the dynamics of the condensate and thermal components of a dilute boson gas. In general, nonadiabaticity should be taken into account when kinetic rates of the system exceed the frequency separations of the excitations relevant to the dynamics of the thermal gas component—for harmonically trapped condensates the latter time scale is given by the trapping frequency. Application of the adiabaticity criterion to a harmonically trapped Bose-Einstein condensate containing an off-axis, precessing vortex line is shown to yield for the vortex velocity a condition which is not fulfilled in the experiments conducted thus far. Deformation of the vortex structure due to its motion is thus suggested to be at least partly responsible for the apparent discrepancies between the predictions of the stationary self-consistent approximations and the results of the vortex precession experiments.

We thank the CSC–Scientific Computing Ltd for computer resources, and the Academy of Finland and the Graduate School in Technical Physics for support.

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