Adiabaticity Criterion for Moving Vortices in Dilute Bose-Einstein Condensates

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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 quasi-particle 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.

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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 fluids. Due to 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 has 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]. 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 the light of the success of the self-consistent approximations in predicting excitation spectra for irrotational condensates [10], 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 quasi-static formalism in describing moving vortices. In order to clarify the latter possibility, we show in this paper that the validity of the quasi-static self-consistent mean-field treatment in modelling moving vortices imposes for the vortex velocity a stringent criterion, which seems to be violated in the precession observations reported so far. This implies that at the observed velocities the quasiparticles can not 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 [11]. Working in the grand-canonical formalism, we start with the Heisenberg equation of motion

\[ i\hbar \frac{\partial}{\partial t} \psi(r, t) = \mathcal{H}_0(r) \psi(r, t) + g \psi(r, t) \psi(r, t) \psi(r, t) \]  

(1)
for the field operator $\psi(r,t)$ of a dilute boson gas. Above, $H_0(\mathbf{r}) \equiv -\hbar^2 \nabla^2 / 2m + V_{tr}(\mathbf{r}) - \mu$ is the grand-canonical one-particle Hamiltonian corresponding to the trapping potential $V_{tr}(\mathbf{r})$ and the chemical potential $\mu$, 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. (3) the Bogoliubov transformation

$$\hat{\psi}(r,t) = \Phi(r,t) + \tilde{\psi}(r,t)$$

(2)

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

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

(3)

for the condensate wavefunction. Above, $\mathcal{L}(r,t) \equiv H_0(r) + 2gn(r,t)$, and

$$n_c(r,t) = |\Phi(r,t)|^2$$

(4a)

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

(4b)

$$n(r,t) = n_c(r,t) + \tilde{n}(r,t)$$

(4c)

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

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

(5)

for the equation of motion of the noncondensate field operator. Substituting into Eq. (3) the Bogoliubov transformation

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

(6)

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

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

(7a)

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

(7b)

Introducing the matrix notations

$$f_n(r,t) = \begin{pmatrix} u_n(r,t) \\ v_n(r,t) \end{pmatrix},$$

$$\mathcal{O}(r,t) = \begin{pmatrix} \mathcal{L}(r,t) & -g\Phi^2(r,t) \\ g\Phi^2(r,t) & -\mathcal{L}(r,t) \end{pmatrix},$$

(8)

(9)

the quasiparticle equations can be expressed in the compact form

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

(10)

For convenience, we also define positive- and negative-sign scalar products of quasiparticle states by setting

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

(11)

here and henceforth, we suppress the arguments of functions when they are not needed for clarity. The requirement that the quasiparticle operators $\alpha_n$, $\alpha_n^\dagger$ 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. (3). This normalization can be straightforwardly verified to be consistent with the TDHFBP equations.

In case the mean fields and, hence, the operator $\mathcal{O}(r,t)$ 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 quasi-stationary eigenequations

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

(12)

This adiabatic approximation is accurate if the transition rates, as determined by the exact time development, of the quasi-stationary states to each other are negligible. In order to formulate this criterion quantitatively, we follow the treatment of Ref. [13]. Let $\{f_i^{(0)}\}$ be a complete set of solutions of Eq. (12); especially, it contains the zero-energy solution $f^{(0)}_0 \propto (\Phi_0, \Phi_0^\dagger)^T$, where $\Phi_0$ is the solution of the stationary GP equation. We orthonormalize the solutions by requiring

$$\langle f_i^{(0)} | f_j^{(0)} \rangle_{-} = \delta_{ij} \quad (i \neq 0); \quad \langle f_0^{(0)} | f_j^{(0)} \rangle_{+} = 1. \quad (13a)$$

In addition, we may impose the condition

$$\langle f_0^{(0)} | f_j^{(0)} \rangle_{+} = 0 \quad (i \neq 0). \quad (13b)$$

In order to analyse the transitions of the quasi-stationary states to each other, we expand the solutions of the TDHFBP equation in terms of them. Substitution of the ansatz

$$f_n(r,t) = \sum_j a_{nj}(t) f_j^{(0)}(r,t) e^{-\frac{i}{\hbar} \int_0^t E_j(\tau') d\tau'}$$

(14)

into Eq. (12) yields the coupled differential equations

$$\sum_j [\hat{a}_{nj} f_j^{(0)} + a_{nj} \hat{f}_j^{(0)}] e^{-\frac{i}{\hbar} \int_0^t E_j(\tau') d\tau'} = 0,$$

(15)
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 (13), and solving for \( a_{n0} \), we find

\[
\dot{a}_{n0} = -\sum_j a_{nj} e^{-\frac{i}{\hbar} \int_0^t [E_j(t') - E_k(t')] dt'} \langle f_0^{(0)} | j_{n}^{(0)} \rangle_+.
\] (16a)

In a similar manner, we derive the equations

\[
\dot{a}_{nk} = -\sum_j a_{nj} e^{-\frac{i}{\hbar} \int_0^t [E_j(t') - E_k(t')] dt'} \langle f_k^{(0)} | j_{n}^{(0)} \rangle_- \] (16b)

for the coefficients corresponding to positive-norm states.

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 rhs of Eqs. (16) as constants, we can integrate them to yield

\[
a_{nk}(t) \approx -\frac{i}{\omega_{nk}} (e^{-i\omega_{nk} t} - 1) \langle f_k^{(0)} | j_{n}^{(0)} \rangle_\pm. \] (17)

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 quasi-stationary states are orthonormalized, the requirement of negligible decay thus implies

\[
\left| \frac{1}{\omega_{nk}} \langle f_k^{(0)} | j_{n}^{(0)} \rangle_\pm \right| \ll 1. \] (18)

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

Consider now the case of a vortex line precessing with frequency \( \nu_\theta \) about a circular orbit of radius \( R_{tr} \) in a harmonically trapped condensate; for simplicity, we assume a trapping potential of the form \( V_{tr} = \frac{1}{2} m \omega_z^2 r^2 \) in cylindrical coordinates \( r = (r, \theta, z) \), and the vortex line to be directed along the \( z \)-axis. 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 (18) for such states, we use the estimate

\[
\langle f_k^{(0)} | j_{n}^{(0)} \rangle_\pm \approx \mathbf{v} \cdot \langle f_k^{(0)} | \nabla f_n^{(0)} \rangle_\pm,
\] (19)

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. (19). Such a system is cylindrically symmetric, and the quasiparticle eigenstates can be chosen to be of the form

\[
u_q(r) = u_q(r) e^{iq_z (2\pi/L) z + i(q_y + 1) \theta}, \] (20a)

\[
u_q(r) = v_q(r) e^{iq_z (2\pi/L) z + i(q_y - 1) \theta}, \] (20b)

where \( q_\theta \) 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

\[
u I_{qq'} \equiv \mathbf{v} \cdot \langle f_q^{(0)} | \nabla f_{q'}^{(0)} \rangle_\pm
\]

\[
\approx -\frac{\mu}{2} \delta_{qq'} \delta_{(q_y + 1)}/| v_q^2 + v_{q'}^2 | \int_0^\infty dr \left[ r \left( u_q \frac{du_q}{dr} \pm v_q \frac{dv_q}{dr} \right) + (q_y - q_\theta) (u_q^2 + v_q^2) \right], \] (21)

where \( \nu = | \mathbf{v} | \) is the magnitude of the velocity of the vortex line, and the states are normalized according to

\[
\int_0^\infty r dr (u_q^2 + v_q^2) = 1, \] (22)

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

We have numerically computed the adiabaticity velocities \( v_{qq'} \) for the lowest excitations of a cylindrical condensate. The static HFB equations were solved self-consistently within the PA and its so-called G1 and G2 variants [12,13], in order to find the quasiparticle amplitudes \( u_q(r), v_q(r) \), and the respective eigenenergies—\( \{q \} \) for details of the methods used in the computations, see Ref. [14]. In order to facilitate comparison with the vortex precession observations, we use parameter values which essentially correspond to the experiments reported in Ref. [15]. Especially, the radial trapping frequency was set to \( \nu_r = \omega_r/2\pi = 7.8 \text{ Hz} \), and the density of the trapped \(^{87}\text{Rb} \) atoms was adjusted to yield a healing length \( \xi = (8\pi n_0 \hbar^2/\mu)^{-1/2} \approx 0.7 \mu\text{m} \) at temperature \( T = 0.8T_{\text{HCC}} \). Here \( n_0 \) denotes the peak density of the condensate, and the condensation temperature \( T_{\text{HCC}} \approx 30 \text{nK} \).

In the experiments, the observed precession radii were of the order of \( R_{pr} \approx R/3 \approx 10 \mu\text{m} \), where \( R \) denotes the radius of the condensate [15]. Bare-core vortices were observed to precess in the direction of the condensate flow with frequency \( \nu_r \approx 1.8 \text{ Hz} \), which corresponds to a velocity \( v_{\text{exp}} = 2\pi R_{pr} \nu_r \approx 0.1 \mu\text{m/s} \). This is to be compared with the computed velocities \( v_{qq'} \) for the lowest
quasiparticle states with $q_z = 0$, displayed in Fig. 1 [4]. Although $v_{\text{exp}} \lesssim v_{qp'}$, we find the adiabaticity condition [3] not to be fulfilled. This suggests that, due to the deformation of the quasiparticle states, the noncondensate can not 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 $(q_x, q_z) = (-1, 0)$, 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 [4]. In fact, this state is almost solely responsible for the differences in the vortex structure between the BA and PA in the low-temperature limit. Deformation of the LCLS due to the vortex motion thus implies crucial modifications for the vortex core structure.

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 (22) 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 $R_{pr}$, via its proportionality to the velocity of the precessing vortex line. In addition, the adiabaticity could depend on the temperature: although we found the smallest $v_{qp'}$ to depend only weakly on temperature, the stationary PA predicts the precession mode frequency and, hence, the precession velocity to have a strong temperature dependence [11].

In conclusion, we have derived a criterion for the validity of the quasi-stationary approximation for a time-dependent mean-field formalism describing the dynamics of the condensate and thermal components of a dilute boson gas. Application of this 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 so 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.

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FIG. 1. The lowest vortex state collective modes with $q_z = 0$, and the adiabaticity velocities $v_{qp'}$ (see Eq. (22)) determined by the transition rates between these states. Note especially the low adiabaticity velocity given by the transitions between the precession (LCLS) and breathing modes. The data corresponds to the PA and system temperature $T \approx 0.8 T_{\text{inc}}$. 
Figure 1