Explaining critical angular velocities of the vortex formation in a stirred Bose-Einstein condensate.

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The problem of explanation of the critical angular velocity \( \Omega_c \) when the formation of a vortex in the stirred Bose-Einstein condensate becomes energetically possible, is considered in the framework of the variational approach. The origin of smallness of the calculated \( \Omega_c \) in comparison with the measured values which takes place for pure quantum state with the unit angular momentum per condensed particle, is uncovered. The agreement with the measured \( \Omega_c \) is achieved upon admitting a small admixture of the zero angular momentum state in the wave function of the one-vortex quantum state prepared after stirring. The portion of this admixture amounts to 10\(\times10^{-13}\%\) of the total condensed atoms. Possible test of this hypothesis is proposed.

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Bose-Einstein condensate (BEC) discovered in the trapped clouds of alkali atoms [1] are proved to be an excellent test site of fundamental concepts of quantum physics of the systems consisting of macroscopically large number of particles [2]. One of the most intriguing features of such systems is the quantized vortex. Recently, the formation of such vortices in the trapped BEC was observed in two different situations. First is the two-component BEC [3], where the vortex state is created via interconversion between two hyperfine states. The second one is realized by the stirring of BEC with the toggled laser beam. This toggling beam creates a small axial asymmetry of the trap potential which is rotated slowly with the angular velocity \( \Omega \). It was found that for \( \Omega \) exceeding a definite critical value \( \Omega_c \), the images of the space distribution of BEC atoms after the ballistic expansion reveals a visible signature of the vortex [4], and even the lattice of the vortex array was observed in some situations [4]. The method of Ref. [4] directly corresponds to the classical experiment with the rotating bucket [5]. As was pointed out in Ref. [4], the measured critical angular velocity of the formation of a single vortex in the stirred BEC appears to be notably larger than that predicted theoretically [6].

Recently, the efforts aimed at explaining larger critical angular velocity were undertaken in Ref. [7]. The purpose of the present note is to propose another explanation of the critical angular velocity \( \Omega_c \) of the stirring of BEC when the formation of the single vortex becomes energetically possible. To this end the energy of different configurations of the BEC atoms is calculated. The reason of smallness of the calculated \( \Omega_c \) as compared to the measured one is revealed. It is shown that the agreement with the measurements can be achieved by assuming the admixture of the vortex-free state with zero angular momentum, in the wave function of the final state prepared after the stirring and containing the visible vortex.

As is known [2], all basic properties of BEC in diluted gases of alkali metals are described by Gross-Pitaevskii (GP) equation [8] which has the form of Schrödinger equation added with the nonlinear term arising due to the short range interaction characterized by the single parameter - the scattering length. Since it is the equilibrium energy of the BEC gas that is of the main concern here, the GP energy functional

\[
E = \int d^3x \left\{ \frac{\hbar^2}{2m} |\nabla \psi|^2 + \frac{m}{2} \left( \omega_\perp^2 r_{\perp}^2 + \omega_z^2 z^2 \right) |\psi|^2 + \frac{2\pi a \hbar^2}{m} |\psi|^4 \right\},
\]

is used instead of GP equation. In the above equation, \( r_{\perp}^2 = x^2 + y^2 \), \( m \) is the mass of an atom, \( \omega_\perp, \omega_z \) are, respectively, the transverse and longitudinal frequencies of the oscillator-like potential modeling the axially symmetric trap, \( a \) is the scattering length. Also, \( \psi \) is the condensate wave function normalized according to the condition

\[
N = \int d^3x |\psi|^2,
\]

\( N \) is the number of condensed atoms. The trap parameters \( N, \omega_\perp, \) and \( \omega_z \) are specified as follows. The first set referred below as the set A is [4].

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\[ N = (1.4 \pm 0.5) \times 10^5, \quad \frac{\omega_\perp}{2\pi} = 219 \text{ Hz}, \quad \frac{\omega_z}{2\pi} = 11.7 \text{ Hz}, \]  
(3)

and the corresponding critical angular velocity of stirring is \( \Omega_c/2\pi = 152 \text{ Hz} \) [8]. The second set referred below as the set B is

\[ N = (3.7 \pm 1.1) \times 10^5, \quad \frac{\omega_\perp}{2\pi} = 171 \text{ Hz}, \quad \frac{\omega_z}{2\pi} = 10.3 \text{ Hz}, \]  
(4)

and the corresponding critical angular velocity of stirring is \( \Omega_c/2\pi = 115 \text{ Hz} \) [8].

Since the accuracy of determination of the number of condensed atoms is about 30 \%, and the energy of BEC is scaled as \( E \propto N^{2/5} \) [see Ref. 8 and Eqs. (7), (11) below], it is unnecessary to bother to calculate \( E \) with the accuracy better than 10\%. So, one may hope that the variational calculation [10] of energy instead of full numerical solution of GP equation will be sufficient. As will soon become clear, it is convenient to take the trial wave function in the form

\[ \psi_\kappa(r_\perp, \phi, z) = \left( \frac{N}{\pi^{3/2} R_\kappa^2 z_\kappa} \right)^{1/2} \left( \sqrt{1 - \kappa^2} + \sqrt{\kappa^2 R_\kappa^2 e^{i\phi}} \right) \exp \left( - \frac{r_\perp^2}{2 R_\kappa^2} - \frac{z^2}{2 z_\kappa^2} \right), \]  
(5)

where 0 \leq \kappa \leq 1; \( R_\kappa \) and \( z_\kappa \) are variational parameters. Notice that \( \kappa = 0, 1 \) corresponds to, respectively, pure vortex-free state and the state with the singly quantized vortex placed at the center of the trap, while intermediate values of \( \kappa \) correspond to arbitrary mixture of the above states. Introducing the dimensionless parameters \( \rho_\kappa \) and \( \zeta_\kappa \) according to the relations \( R_\kappa = (\hbar/m\omega_\perp)^1/2 \rho_\kappa \) and \( z_\kappa = (\hbar/m\omega_z)^1/2 \zeta_\kappa \), one can find from Eqs. (1) and (5) the energy per condensed atom:

\[ E(\kappa) = \frac{\hbar \omega_\perp}{2} \left( \frac{1}{\rho_\kappa^2} + \rho_\kappa^2 \right) (1 + \kappa) + \frac{\hbar \omega_z}{4} \left( \frac{1}{\zeta_\kappa^2} + \zeta_\kappa^2 \right) + \frac{\hbar \omega_\perp \gamma_z}{\rho_\kappa^2 \zeta_\kappa} \left( 1 - \frac{\kappa^2}{2} \right), \]  
(6)

where

\[ \gamma_z = aN \left( \frac{m\omega_z}{2\pi\hbar} \right)^{1/2}. \]  
(7)

The mean value of angular momentum in the quantum state with the wave function Eq. (5) is

\[ \langle L_z \rangle = \int d^3x \psi_\kappa^* \left( -i\hbar \frac{\partial}{\partial \phi} \right) \psi_\kappa = \hbar N \kappa. \]  
(8)

As is known [3,11], the condition of thermodynamic possibility of the vortex formation in the system rotated at the angular velocity \( \Omega \) can be formulated as \( \Delta E - \langle L_z \rangle \Omega < 0 \), where \( \Delta E \) is the energy difference between the states with vortex and without it, so that the critical angular velocity is defined as \( \Omega_c = \Delta E / \langle L_z \rangle \). Let us evaluate \( \Omega_c \) in the framework of variational approach.

The values of variational parameters \( \rho_\kappa \) and \( \zeta_\kappa \) can be found from the condition of the minimum of the BEC energy Eq. (8) which is reduced to the following equations:

\[ \rho_\kappa^2 - \rho_\kappa^{-2} = \frac{2 \gamma_z (1 - \kappa^2/2)}{\rho_\kappa^2 \zeta_\kappa (1 + \kappa)}, \]

\[ \zeta_\kappa^2 - \zeta_\kappa^{-2} = \frac{2 \omega_\perp \gamma_z (1 - \kappa^2/2)}{\omega_z \rho_\kappa^2 \zeta_\kappa}. \]  
(9)

First, let us consider the problem of the critical angular velocity in the approximation when the kinetic energy of both the transverse and longitudinal motion can be neglected. This is the Thomas-Fermi (TF) limit [12]. The solution of Eq. (8) in this limit looks as

\[ \rho_\kappa^{TF} = \left[ \frac{4 \gamma_z^2 \omega_z (1 - \kappa^2/2)^2}{(1 + \kappa)^3 \omega_\perp} \right]^{1/10}, \]

\[ \zeta_\kappa^{TF} = \rho_\kappa^{TF} \left[ \frac{\omega_\perp}{\omega_z (1 + \kappa)} \right]^{1/2}. \]  
(10)

Direct numerical evaluation shows that at, say, \( \kappa = 0 \) the parameters \( \rho_0^{TF} = 2.16 \) (2.63) and \( \zeta_0^{TF} = 9.36 \) (10.7) evaluated in this limit for the set of parameters Eq. (8) [respectively, (9)], coincide within the accuracy 1\% with those
found from Eq. (10). Hereafter, when doing the specific numerical evaluations, we take the scattering length $a = 5.77$ nm for $^{87}$Rb atoms [12], and the above two sets of BEC parameters from Eqs. (3) and (4). The corresponding energy in TF limit is found to be

$$E_{\text{TF}}^N(\kappa) = \frac{5}{4} \hbar \omega_{\perp} \left( \frac{4 \gamma^2 \omega_z}{\omega_{\perp}} \right)^{1/5} \left[ (1 + \kappa)(1 - \kappa^2/2) \right]^{2/5}.$$  \tag{11}

One can see that in TF limit the energies of pure vortex-free state ($\kappa = 0$) and the state with the single vortex ($\kappa = 1$) are equal, hence $\Omega_c$ found from relation

$$\frac{\Omega_c(\kappa)}{2\pi} = \frac{E(\kappa) - E(0)}{2\pi \hbar N \kappa},$$  \tag{12}

[see 2 and Eq. (8)], at $\kappa = 1$, vanishes in TF limit. Thus, one should take the kinetic energy of the BEC cloud into account. Here this is done by the numerical solution of Eq. (9) for the two values $\kappa = 0, 1$. The result is $\rho_0 = 2.19 (2.64)$, $\zeta_0 = 9.28 (10.66)$, and $\rho_1 = 1.61 (1.90)$, $\zeta_1 = 9.06 (10.53)$, in the case of the experimental conditions Eq. (3), (4), respectively. One then finds $\Omega_c^A/2\pi = 65.9$ Hz, and $\Omega_c^B/2\pi = 36.1$ Hz, where upper indices refer to the two above sets of the trap parameters. The smallness of these values as compared to the experimentally measured is due to smallness of the energy difference between the pure BEC states with $\kappa = 0$ and 1.

To reconcile the result of calculations with the measurements in the present approach, one should have in mind that, in fact, the density of atoms does not vanish in the central dip [4]. The authors of Ref. [4] propose three possible reasons for this: (i) oscillations of the vortex filament, (ii) the presence of non-condensed atoms, and (iii) insufficient resolution of the imaging optics as compared to the vortex core radius of the BEC cloud. Here we propose the fourth possible reason and admit that the quantum state of the BEC cloud after the stirring is the superposition of pure quantum states with the angular momenta per particle $L_z/N = 0$ and $\hbar$, that is, admitting $\kappa \neq 1$ in the wave function Eq. (9) of final quantum state. The presence of BEC atoms in the state with zero angular momentum explains in a natural way a nonzero density in the central dip.

Solving Eq. (8) numerically, one can find the energy dependence on $\kappa$ and calculate the critical angular velocity from Eq. (12). The result of this calculation is shown in Fig. 1. Then fitting the calculated critical angular velocity $\Omega_c$ to the experimental values is possible if the portion $\kappa^A$ of the number of BEC particles in the state with the unit angular momentum per particle amounts to, respectively,

$$\kappa^A = 0.87, \quad \kappa^B = 0.90.$$  \tag{13}

The latter values, in view of Eq. (8), give $(L_z)/N = 0.87\hbar$, respectively, $0.9\hbar$, and do not contradict to the measured magnitude [3] of the mean angular momentum of the condensate. Eq. (13) means that the admixture of the atoms in the zero angular momentum state in the case of the trap parameters Eq. (3) [4] amounts to 0.13 (0.1), respectively. Notice that despite essential difference in the experimental trap parameters Eqs. (3) [4] and (4) [3], the portion of the number of atoms in the zero momentum state needed to explain very different observed critical angular velocities in the final state prepared after the stirring, turns out to be practically same. To be more precise, the 30 % accuracy of the determination of the number of atoms in the condensates reported in Refs. [3] implies, as is explained earlier in this paper, approximately 10% uncertainty of the calculation of energy per condensed atom which is translated to approximately the same uncertainty of calculation of $\kappa$, while the central values of the calculated $\kappa$ differ in the above experimental conditions by 3 – 4%, which is well below their estimated uncertainty.

Could such proposed feature of the BEC wave function as the presence of the portion $1-\kappa$ of zero angular momentum condensed atoms be tested in experiments? Let us discuss this issue. As is known [11], the presence of the vortex is detected through the visualization of the images of BEC cloud obtained after its ballistic expansion. One can obtain the spatial distribution of the BEC atoms after this expansion with the usual quantum mechanical method upon finding the wave function Eq. (9) in the momentum space form, propagating it forward in time freely, then finding its resulting coordinate space form. The resulting spatial distribution appears to be

$$\rho(r_\perp, \phi, z, t) = \frac{N}{\pi^{3/2} R_{\kappa}^{3/2} z^{3/2}} \left( 1 + \frac{\hbar^2 t^2}{m^2 z^{3/2}} \right)^{-1/2} \left( 1 + \frac{\hbar^2 t^2}{m^2 R_{\kappa}^2} \right)^{-1} \exp \left[ -\frac{r_\perp^2}{R_{\kappa}^2 + \left( \frac{\hbar t}{m z_{\kappa}} \right)^2} - \frac{z^2}{z^2 + \left( \frac{\hbar t}{m z_{\kappa}} \right)^2} \right] \times$$

$$\times \left[ 1 - \kappa + \frac{\kappa r_\perp^2}{R_{\kappa}^2} + 2 \sqrt{\kappa(1-\kappa)} r_\perp \left( \cos \phi + \frac{\hbar t}{m R_{\kappa}} \sin \phi \right) / R_{\kappa} \right].$$  \tag{14}
One can see that the dependence of the spatial distribution of the BEC atoms on the azimuth angle $\phi$ is the signature of the above admixture of the vortex free state. The dependence arises from the interference term. But the contribution of the latter becomes significant only after some time of duration of the process of free expansion. Taking the estimates of the root mean squared values of $r_\perp/R_\kappa$ and $r_\perp^2/R_\kappa^2$ from the written spatial distribution function, one can find that the axial asymmetric contribution $\propto \sin \phi$ becomes to dominate after the time of flight

$$t > \tau \approx \frac{m R_\kappa^2}{\hbar} \sqrt{\frac{\kappa}{2(1 - \kappa)}}.$$  \hfill (15)

Using the parameter sets Eqs. (3), \(|(4)|\), and the results of numerical solutions of Eq. (9) together with Eq. (13), one can find from Eq. \(|13|\) that the interference term becomes to dominate after the free expansion time exceeding $\tau = 24$ ms (50 ms), respectively. Since the time of free expansion reported in Refs. \(|4|,|9|\) is 27 ms, it is clear that the proposed feature of the final wave function that could emerge after the stirring has not enough time to develop in the experiments \(|4|,|9|\). An additional testable feature of the proposed wave function of the final state is the flattening of the central vortex dip in the density distribution due to the increasing relative contribution of the zero angular momentum state $\propto 1 - \kappa$ as time of free expansion of the BEC cloud is increasing. It would be interesting to enlarge (if possible) the time of ballistic expansion of the BEC clouds after the stirring to see if the dependence of their spatial distribution will acquire the angular dependence $\propto \sin \phi$, and to study the relative weights of the components of condensed atoms with different angular momentum at different times of their ballistic expansion.

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FIG. 1. The dependence of the critical angular velocity of formation of the quantum state of BEC with one vortex on the portion $\kappa$ of atoms in the state with the unit angular momentum per particle. The curves labeled by A and B correspond to the trap parameters Eq. (3) and (4), respectively.