Rotating Bose-Einstein Condensates with a large number of Vortices.

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We study a harmonically-confined Bose-Einstein condensate under rotation. Vortex lattice configurations are investigated through a variational approach. Vortices with more than a unit of angular momentum are not stable. We explicitly show that the critical rotational frequency is quite small, as was reported in the MIT experiment. The width of the condensate in the xy plane and along z, and the vortex density are determined as functions of the rotational frequency. The aspect ratio becomes small for large rotational frequencies, making the condensate an effectively two-dimensional system.

In recent experiments \[1,2\], a large number of vortices (about 150) have been generated in a Bose-Einstein condensate of Na atoms. The vortices form a hexagonal lattice, in a quasi equilibrium, showing a variety of properties which differ from an equilibrium system. In these experiments, a large angular momentum is imparted to the condensate by rotating it close to the quadrupolar frequency. In addition, the condensate is subjected to an asymmetric harmonic confining potential: \(\omega z/2\pi \sim 20Hz\), \(\omega xy/2\pi \sim 80Hz\), the rotation axis being along \(z\) in the MIT experiment \[1\]. The high angular momentum states of the Bose condensate are similar to the quantum Hall systems and type-II superconductors. If the rotational frequency \(\Omega\) is exactly same as in-plane harmonic frequency \(\omega xy\), these states can be mapped to the lowest Landau level of quantum Hall systems \[3\].

The angular momentum that is transferred to the condensate is carried by vortices, each vortex carrying a quantum of angular momentum, similar to the vortices in a superfluid. The vortices have an effective repulsion, which we shall see later from a variational calculation. This implies that a vortex with two quanta of angular momentum is unstable against separating into two unit vortices. When a large angular momentum is deposited on the condensate, the vortices form a regular lattice in the xy plane. The unit cell area \(\nu\) of the vortex lattice will depend on the rotational frequency, the harmonic frequencies, and the two-particle scattering length of Na atoms, through the parameters characterizing the condensate wavefunction. In the previous work of Ho \[3\], the energy of the vortex lattice has been calculated through a variational approach within the Gross-Pitaevskii paradigm, using a Thomas-Fermi approximation. The calculated critical rotational frequency does not agree with the MIT experiment \[1\]. We will carry out a variational calculation, with a variational condensate wavefunction that is similar to the one used in \[3\], that allows us to estimate the critical rotational frequency which is in excellent agreement with the experiment, and the aspect ratio of the condensate (the ration of the rms widths in the xy plane and along the z-direction).

The condensate wavefunction is determined from minimizing the Gross-Pitaevskii functional \[3\]

\[
K = \int \psi^* [H_{xy} - \Omega L_z + H_z] \psi d^3r + \frac{gN}{2} \int |\psi|^4 d^3r \tag{1}
\]

where the single-particle Hamiltonians along \(z\) and in the \(xy\) plane are

\[
H_z = \frac{\hbar^2}{2m} \nabla_z^2, \quad H_{xy} = -\frac{\hbar^2}{2m} \nabla_{xy}^2 (x^2 + y^2); \quad L_z = \text{the angular momentum along } z \text{ direction along which the condensate is rotated with a frequency } \Omega; \text{ the two-particle interaction strength is } g = 4\pi \hbar^2 a_{sc}/M \text{ in terms of the s-wave scattering length}; \quad N \text{ is the number of atoms in the condensate, and } M \text{ is the mass of the Na atom. The wavefunction } \psi \text{ is normalized to unity. The Hamiltonian in the xy plane is similar to that of a charged particle in a magnetic field if } eB/Mc = 2\omega xy, \text{ at } \omega xy = \Omega. \text{ In this case the energy levels are Landau levels, with the lowest level degenerate for angular momentum quantum number } m = 0, 1, 2. \text{ The degeneracy gets lifted for } \omega xy \neq \Omega.

In the absence of interactions, for \(g = 0\), the lowest energy state is a direct product of harmonic oscillator wavefunctions along \(z\) direction and in the \(xy\) plane, with uniform densities (modulo the gaussian variation). However, for \(g \neq 0\), states with nonuniform densities, more specifically with density vanishing at points signifying vortices, are favorable. These states will become stable for \(\Omega > \Omega_c\), where \(\Omega_c\) is the critical rotational frequency. We will follow in spirit \[3\] to estimate the critical rotational frequency. Let us write \(\psi(r, z) = \Phi_m(r)\chi(z)\), by separating the \(z\) direction and \(xy\) plane, where \(\chi(z) = c_z \exp(-z^2\gamma^2/2a_z^2)\), \(\Phi_m(r) = c_m \exp(\gamma r^2/2a_z^2)\); \(a_z = \sqrt{\hbar/M \omega z}\) and \(a_{xy} = \sqrt{\hbar/M \omega xy}\) are the oscillator lengths, \(\gamma, \beta\) are variational parameters, and \(c_m, c_z\) are normalization constants. The wavefunction carries an angular momentum \(m\), and since \(|\Phi|^2 \sim r^{2m}\), it also signifies a vortex at the origin of strength \(m\). For \(\Omega = 0\), the uniform density state (modulo a gaussian variation), viz. \(m = 0\) has the lowest energy for \(\gamma = 1, \beta = 1\) in the absence of the interactions, corresponding to the groundstate of the harmonic oscillator. For \(g \neq 0\), the parameters \(\beta, \gamma\) will change substantially. The energy of the configuration \(\Phi_m\) is (in units of the oscillator energy \(\hbar \omega xy\))

\[
K_m = \left\{ \frac{1}{2} \left( \frac{1}{\beta^2} + \beta^2 \right) - \frac{\Omega}{\omega xy} \right\} I_1 + \frac{\omega z}{4 \omega xy} \left( \frac{1}{\gamma^2} + \gamma^2 \right)
\]
where the dimensionless parameter $G = N\alpha_{sc}/a_c\sqrt{2\pi}$ (using experimental values $N = 5 \times 10^7$, $\alpha_{sc} = 50$ Bohr radii, $a_c = 0.9 \times 10^{5}$ Bohr radii, the interaction strength is $G \sim 1.1 \times 10^4$). The coefficient of the first term in the above equation, $\Gamma_1 = r^2 > \beta^2/\omega_{xy}^2$, is just the rms width of the wavefunction in units of $a_x^2/\beta^2$; $\Gamma_1(m) = m + 1$. The coefficient of the last term, $\Gamma_2 = 2\pi a_x^2/\beta^2 \int |\Phi|^4$, is the interaction contribution; $\Gamma_2(m) = 2m!/(m+1)2m$. Minimizing the energy w.r.t. parameters $\gamma$ and $\beta$ for the cases of $m = 0$ (no vortex configuration) and $m = 1$ (one vortex of unit strength), we obtain $\gamma_0 = \gamma_1 = (\omega_z/\omega_{xy})^{2/5}(2G)^{-1/5}$, $\beta_0^2 = \gamma_0^2(\omega_{xy}/\omega_z)$, $\beta_1^2 = 2\beta_0^2$. For the experimental values of $\omega_z/\omega_{xy} = 1/4$, $G = 10^4$ we get $\gamma_0 = 0.08, \beta_0 = 0.16$ (in contrast, $\gamma = \beta = 1$, when $g = 0$ for the no-vortex state). And the energy difference between the two configurations

$$K_1 - K_0 = \frac{3\gamma_0^2\omega_{xy}}{\omega_z} - \frac{\Omega}{\omega_{xy}} \equiv \frac{\Omega_c - \Omega}{\omega_{xy}}$$

will be negative for $\Omega > \Omega_c$, where the critical rotational frequency is $\Omega_c/\omega_{xy} = 3\gamma_0^2\omega_{xy}/\omega_z$ is about 0.077 for the experimental values of $G = 10^4$, $\omega_z/\omega_{xy} = 1/4$. This compares very well with the MIT experiments [1], where vortices have been observed for frequencies as low as 7 Hz, with the harmonic oscillator frequency of 80 Hz.

The above discussion establishes that for $\Omega > \Omega_c$ vortex configurations are stable against a uniform density state. We examined configurations with larger strength of vortex, viz. for $m = 2, 3, ...$. A larger $m$ will lower the interaction term, which is clear from the coefficient, but will increase the rms width of the wavefunction. For $m = 2$, the energy is minimized for $\gamma_2 = \gamma_0(8/9)^{1/5}$, and $\beta_2^2 = 2\beta_0^2(6/5)$, implying $K_2 - K_1 = 1.25\gamma_0^2((8/9)^{2/5} - 1)\omega_z/\omega_{xy} > 0$. It can be seen that for $m > 2$, the energy is not favorable, implying a vortex with angular momentum larger than one unit is not stable. The $m = 2$ state is unstable against a state with two $m = 1$ vortices separated by some distance. The energy is lower for a larger separation, implying an effective repulsion between the vortices. We can investigate states with a large angular momentum by looking at configurations with a large number of vortices with unit strength. This is tantamount to separating the vortices in state $\Phi_m$. Instead of a m-vortex sitting at the origin, we will have m vortices spread all over. The effective repulsion between the vortices gives a finite spacing. A regular lattice structure is easily probed, either triangular or rectangular (the only Bravais lattices in two dimensions).

Let us consider a trial wavefunction [3], with $q$ vortices each carrying a unit of angular momentum

$$\Phi = c_q e^{-r^2/2a_x^2} \prod_{l=1}^{q} (z - z_l) = \sum_{m=0}^{q} x_m \Phi_m$$

where we introduce a vortex function $f(z) = \prod(z - z_l)$. $z_l = x_l + i y_l$ is the complex coordinate of the lth vortex (carrying a unit of angular momentum). We have also written the wavefunction as a superposition of various configurations $\Phi_m$ (carrying one vortex of strength $m$). Noting that $\int \Phi_m H_{xy} \Phi_m = 0$, for $m \neq m'$, the energy of this state can be written as before (Eq.2) with

$$\Gamma_1 = \frac{\beta^2}{a_x^2} \int |\Phi|^2 r^2 d^2 r$$

and

$$\Gamma_2 = \frac{2\pi a_x^2}{\beta^2} \int |\Phi|^4 d^2 r.$$  

The evaluation of the above coefficients $\Gamma_1, \Gamma_2$, is quite involved, as the computation of the integrals is not straightforward, because of the presence of the vortex function $f(z)$. We shall try to extract the leading order behaviour of these coefficients as functions of the ratio $\pi a_x^2/\beta^2 \nu$, where $\nu$ is the unit cell area of the vortex lattice.

Firstly, we note that the vortex function can be written as $f(z) = z(z^6 - b_n^6)(z^6 - b_n^6)(z^6 - b_n^6)(z^12 - b_n^{12})...$, for a triangular lattice (actually a hexagonal lattice, including the z direction) where $b_n$ is the $n$th neighbor distance in units of $a_x/\beta$. Each $b_n$ occurs with a power which is equal to the coordination number of the $n$th neighbor vortex. For triangular lattice the coordination is either 6 or 12. In the case of a square lattice the coordination number is either 4 or 8. Here we have fixed the origin on one of the vortices. In the product $(z - z_1)...(z - z_6)$ of the first neighbor vortices, only two terms are nonzero, viz. $z^6, z_1 z_2...z_6 = -b_n^6$. Similarly for the other neighbour vortices. We now resort to a simple approximation to estimate $f(z)$. Let us write

$$\log f(z) = \sum_{\nu} \log(z - z_i) = \frac{1}{\nu} \int_0^R r^2 dr^2 \int_{2\pi} |d\theta \log(z - r e^{i\theta})|,$$

where we replaced the sum by an integral, and $\nu$ is the unit cell volume of the vortex lattice. In the above approximation, namely replacing the density of vortices by a constant, we have ignored the finite-size corrections that arise, as the lattice size is not too big (about 150 vortices or less). This approximation is similar to the average-vortex approximation of [3]. The details of finite-size effects on the vortex function will be given elsewhere. Here, we will keep only the smooth part of the density of vortices. In the integral the upper limit, viz. the size of the vortex lattice, is taken to be $R$, with $\pi R^2/\nu = q$, the total number of vortices. The integral is easily done, by doing an integration by parts in $r^2$ variable, keeping the log function as the second function, we get (using $|z| = r$)

$$\log f \approx i q \pi + \log(\frac{q \nu}{\pi})^{q^2/2} + \frac{\pi a_x^2}{2\nu}.$$

\[2\]
Now, \( |f(z)|^2 = (q
u/π)^4 \exp(\pi r^2/\nu) \), and in turn the condensate density is given by

\[
|\Phi|^2 = |c_q|^2 \left(\frac{q\nu}{\pi}\right) e^{-r^2/2(1-\alpha)} e^{-2\nu^2}, \quad \alpha = \frac{\pi a_{xy}^2}{\nu \beta^2}.
\]  

(8)

In the above, \( \alpha \) is the ratio of the area of the effective Larmor circle and the unit cell area of the vortex lattice. In Fig.1 we plot the numerically computed function \( \log |f|^2 \) for a lattice with 145 sites, along with the approximate value that we calculated by doing an integral. As can be seen from the figure, the above computation (Eq.7) is in excellent agreement with the numerical computation, implying the finite-size effects are quite small here.

The total condensate density \( |\Phi|^2 \) has now three variational parameters, namely, \( \alpha \) the number of vortices in an effective Larmor circle, \( \beta \) the inverse rms width in the xy plane, \( \gamma \) the inverse rms width along z direction. The coefficients \( \Gamma_1, \Gamma_2 \) are calculated as

\[
\Gamma_1 = \frac{1}{1-\alpha}, \quad \Gamma_2 = 1 - \alpha.
\]

In the limit of \( \alpha \to 0, \Gamma_1 = \Gamma_2 = 1 \), we have the no vortex state. Now, our task is to minimize the Gross-Pitaevskii energy (Eq.2) over variation of the parameters \( \alpha, \beta, \gamma \). Setting the derivatives of \( K(\alpha, \beta, \gamma) \) w.r.t. the three variational parameters to zero, we obtain

\[
\frac{1}{2} \left( \frac{1}{\beta^2} + \beta^2 \right) - \frac{\Omega}{\omega_{xy}} = G \gamma \beta^2 (1 - \alpha)^2 \quad \text{(9)}
\]

\[
\frac{1}{2} \left( \frac{1}{\beta^2} - \beta^2 \right) = G \gamma \beta^2 (1 - \alpha)^2 \quad \text{(10)}
\]

\[
\frac{\omega_z}{2 \omega_{xy}} \left( \frac{1}{\gamma^2} - \gamma^2 \right) = G \gamma \beta^2 (1 - \alpha) \quad \text{(11)}
\]

The first two equations imply \( \beta^2 = \Omega/\omega_{xy} \), and the last two imply

\[
\left( \frac{1}{\gamma^2} - \gamma^2 \right)^2 = 2G \gamma (1 - \beta^4) \frac{\omega_{xy}^2}{\omega_z^2}.
\]

In the limit of \( \Omega \to \omega_{xy}, \beta^2 \) tends to one, and \( \gamma \) will also approach unity, as can be seen from the above equation. However, even for \( \Omega/\omega_{xy} = 0.9 \), the right hand side of the equation is quite large (because \( G = 10^4, \omega_{xy}/\omega_z = 4 \)), implying \( \gamma \) is quite small. Here, we can approximate \( \frac{1}{\gamma^2} - \gamma^2 \approx \frac{1}{\gamma^2} \) (this is tantamount to dropping the kinetic energy term in \( H_z \) (Eq.1), as usually done in the Thomas-Fermi approximation \([3]\), and thus obtain (valid for \( \Omega > \Omega_c \))

\[
1 - \alpha = \frac{(1 - \beta^4)^{5/2}}{\beta^2 (2G)^{3/2}} (\frac{\omega_{xy}}{\omega_z})^{5/2}, \quad \beta^2 = \frac{\Omega}{\omega_{xy}}
\]

\[
\gamma = \frac{\omega_z}{\omega_{xy}} \frac{1}{(2G)^{3/2} (1 - \beta^4)^{3/2}}.
\]

As \( \Omega \to \omega_{xy}, \beta^2 \to 1, \alpha \to 1 \), which would imply \( \gamma \to 1 \), which implies the rms width along z direction will tend to \( a_z \). In the neighborhood of \( \Omega \leq \omega_{xy} \), \( \gamma \) has the form shown in the above equation. Similarly, as \( \Omega \to 0, \beta^2 = \beta_0^2 = 0.16, \gamma = \gamma_0 = 0.08, \alpha = 0 \). The rms widths of the condensate in the xy plane, and along z direction are

\[
R_{xy} = \sqrt{<r^2>} = \frac{a_{xy}}{\beta \sqrt{1 - \alpha}}, \quad R_z = \sqrt{<z^2>} = \frac{a_z}{\sqrt{2\gamma}}.
\]

In the quantum-Hall limit (\( \Omega = \omega_{xy} \)), the unit cell area of the vortex lattice becomes \( \nu = \pi a_{xy}^2 \), implying as many vortices as the number of particles in the condensate. The width of the condensate becomes very large in the xy plane, and the width along z direction becomes very small (and saturates at \( a_z/\sqrt{2} \)), as can be seen from the above relations.

Table 1: For various values of the rotational frequency, the number of vortices within a size of the rms width of the condensate density, the rms width of the condensate in the xy plane, and the rms width along z direction. We have used the experimental values of \( G = 10^4 \), and \( \omega_{xy}/\omega_z = 1/4 \). Note that within a size of 1.5\( R_{xy} \) (the condensate density falls to 10 per cent) the number of vortices is 2.25 times that shown in the second column; for example the number of vortices in the condensate is effectively about 25 for the second case shown. As \( \Omega \) increases the rms width along z direction decreases, which will saturate at \( a_z/\sqrt{2} \) in the limit \( \Omega \to \omega_{xy} \).
The optimal Gross-Pitaevskii energy is given by

\[ \frac{1}{\nu} = \frac{\alpha \beta^2}{\pi a^2_{xy}} = \frac{2M\Omega}{\hbar} \alpha \]

which reduces to the familiar \( 1/\nu = 2M\Omega/\hbar \) in the limit of \( \Omega \to \omega_{xy} \). The optimal number of vortices within a size of the rms width of the condensate is

\[ \frac{\pi < r^2 >}{\nu} = \frac{\alpha}{1 - \alpha} \].

The optimal Gross-Pitaevskii energy is given by

\[ K = \frac{5}{4 \pi^2} \frac{2}{N} \left( \frac{\omega_z}{\omega_{xy}} \right)^\frac{1}{2} \left( \frac{a_{xy}}{a_z} \right)^\frac{3}{2} (1 - \frac{\Omega^2}{\omega_{xy}^2})^\frac{3}{2} \hbar \omega_{xy}. \]

In Table 1 we have listed the optimal values of the variational parameters, the rms widths, the number of vortices within the rms width, for various values of the rotational frequencies. These results are different from the work of [3]. For \( \Omega/\omega_{xy} \sim 0.9 \), there are a large number of vortices, and \( \gamma \) is still small, the density profile along \( z \) direction is similar to the inverted parabola of [3], except near the edge where it has a gaussian tail. But, as \( \Omega \) becomes closer to \( \omega_{xy} \), as \( \gamma \to 1 \), the density profile along \( z \) direction is that of the harmonic oscillator groundstate (the rms width is equal to \( a_z \)). A quantitative measure of how far the system is from quantum-Hall limit can be taken as \( 1 - \gamma \).

In the foregoing analysis, the leading order behaviour is valid for \( \Omega \sim \omega_{xy} \), where a large number of vortices are generated. The lattice structure of the vortices enters only through the density. The triangular lattice is favored over the square lattice, as for the same density of vortices (\( \nu = \sqrt{3}c_{tr}/2 = c_{sq}^2 \), where \( c_{tr}, c_{sq} \) are the lattice spacing for the triangular and square lattices respectively), the spacing is larger in the case of triangular lattice. Since the vortices have an effective repulsion, a larger spacing is favored for energy minimization. But, in the quantum-Hall regime (\( \Omega = \omega_{xy} \)), the energies of the two lattice structures become degenerate (square lattice energy approaches that of the triangular lattice from above). Then it becomes important to consider all perturbations, though small and hence hitherto neglected, to lift the degeneracy to find the true groundstate configuration. This implies one should go beyond the Gross-Pitaevskii for the condensate wavefunction. There is also a possibility of formation of higher angular momentum vortices (for \( \Omega > \omega_{xy} \)), and maybe an instability of fragmenting of the condensate. This is because, once the unit cell area becomes equal to the area of Larmor circle, the angular momentum that can be carried by \( m = 1 \) vortices gets saturated. If a larger angular momentum is transfered to the system, \( m > 1 \) get generated, or the system breaks into smaller pieces. It will be interesting to investigate other variational states in this regime, as the physics here is similar to that of a Quantum Hall system. We are investigating these issues currently, along with the question of multi-component Bose condensates where the internal degree of freedom introduces many features motivating many novel variational states.

In conclusion, we have calculated the critical rotational frequency \( \Omega_c/\omega_{xy} \sim 0.07 \), above which vortices become stable, which compares very well with the MIT experiments. We have shown that variational states, with a gaussian density profile along \( z \) direction, and density profile with vortices of unit strength, the locations forming a triangular lattice, in the xy plane get stabilized for larger \( \Omega \). We have computed the width of the wavefunctions along \( z \) direction, and in the xy plane, the aspect ratio becoming very small as \( \Omega \to \omega_{xy} \). The unit cell area of the vortex lattice becomes equal to the Larmor circle area in this limit, implying as many vortices as the number of condensate atoms.

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