Landau levels and the Thomas-Fermi structure of rapidly rotating Bose-Einstein condensates

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(Dated: July 14, 2021)

We show that, within mean-field theory, the density profile of a rapidly rotating harmonically trapped Bose-Einstein condensate is of the Thomas-Fermi form as long as the number of vortices is much larger than unity. Two forms of the condensate wave function are explored: i) the lowest Landau level (LLL) wave function with a regular lattice of vortices multiplied by a slowly varying envelope function, which gives rise to components in higher Landau levels; ii) the LLL wave function with a nonuniform vortex lattice. From variational calculations we find it most favorable energetically to retain the LLL form of the wave function but to allow the vortices to deviate slightly from a regular lattice. The predicted distortions of the lattice are small, but in accord with recent measurements at lower rates of rotation.

PACS numbers: 03.75.Hh, 05.30.Jp, 67.40.Vs, 67.40.Db

How very rapidly rotating Bose-Einstein condensates carry angular momentum remains a fundamental question of many-particle physics. Ho\textsuperscript{[1]} noting that the Hamiltonian for a rotating gas in a harmonic trap is similar to that for charged particles in a magnetic field, argued that for rotational angular velocities just below the Coriolis force. Motivated by this insight, Schweikhard et al.\textsuperscript{[2]} (following earlier work in \textsuperscript{[3]}) have recently achieved rotational angular velocities $\Omega$ in excess of $0$ following earlier work in \textsuperscript{[3]} have recently achieved rotational angular velocities $\Omega$ in excess of $0$. This effect comes about through a modification, with increasing $g_{n_{\perp}}$ of the condensate wave function, $\Psi$, from $N^{1/2}\phi_{\text{LLL}}^0$. A modification of $\Psi$ that allows the density distribution to spread out tends to reduce the interaction energy: for infinitesimal modification, $\Psi \sim \phi_{\text{LLL}}^0 + \delta \Psi$, the change in the interaction energy is linear in $\delta \Psi$, and, with the proper choice of the phase of $\delta \Psi$, is negative. Such modification costs kinetic and trap energy, which however is quadratic in $\delta \Psi$ for infinitesimal modification. Thus the state $\Psi^0$ for a uniform array of vortices is always unstable towards smoothing out of the density distribution. The resulting change in the density profile can be

\begin{equation}
\phi_{\text{LLL}}(r) = A_{\phi} \prod_{i=1}^{N} (\zeta - \zeta_i) e^{-r^2/2d_{\perp}^2},
\end{equation}

where the rotation axis is along $\hat{z}$, $\zeta = x + iy$, the $\zeta_i$ are the vortex positions, $r = (x, y)$, $d_{\perp} \equiv \sqrt{h/m\omega_{\perp}}$ is the transverse oscillator length, and the constant $A_{\phi}$ normalizes $\int d^2r |\phi_{\text{LLL}}|^2$ to unity – Ho predicted that for a uniform lattice (at each height), the smoothed density profile of a trapped cloud would be Gaussian:

\begin{equation}
\langle |\phi_{\text{LLL}}^0|^2 \rangle = \frac{1}{\pi \sigma^2} e^{-r^2/\sigma^2}.
\end{equation}

Here the superscript “u” denotes that the vortex density is uniform, $1/\sigma^2 = 1/d_{\perp}^2 - \pi n_{\perp} \sigma$, $n_{\perp}$ is the vortex density in the plane perpendicular to the rotation axis, and $\langle \ldots \rangle$ denotes an average over an area of linear size large compared with the vortex separation but small compared with $\sigma$. On the other hand, Ref. \textsuperscript{4} – adopting a more general wave function, as in \textsuperscript{5}, that is a product of a slowly varying envelope describing the global structure of the cloud and a rapidly varying function describing the local properties of individual vortices – found that for a uniform array of vortices and for $N_{a_{\perp}}/Z \gg 1$, where $Z$ is the height in the $z$ direction, the density profile is a Thomas-Fermi (TF) inverted parabola. In current experiments \textsuperscript{2}, $N_{a_{\perp}}/Z$ is of order 10-100, and the transverse density distributions are in fact better fit with a TF profile than a Gaussian. Theoretical evidence for the Thomas-Fermi profile has previously been found in numerical studies \textsuperscript{6}.

As first pointed out by A.H. MacDonald (see Ref. \textsuperscript{37} of \textsuperscript{7} and stressed to us by N. Read \textsuperscript{8}, one can achieve significant changes in the density while maintaining a condensate wave function made only of LLL components, if one allows the vortex lattice to relax from exactly triangular, an effect not considered in Refs. \textsuperscript{1} \textsuperscript{4}. We show here that when the lattice is permitted to relax only slightly from uniformity, the TF form is generally obtained for $N_{a_{\perp}}/Z \gg 1 - \Omega/\omega_{\perp}$. Thus TF behavior extends to much lower densities than previously realized. This effect comes about through a modification, with increasing $g_{n_{\perp}}$ of the condensate wave function, $\Psi$, from $N^{1/2}\phi_{\text{LLL}}^0$. A modification of $\Psi$ that allows the density distribution to spread out tends to reduce the interaction energy: for infinitesimal modification, $\Psi \sim \phi_{\text{LLL}}^0 + \delta \Psi$, the change in the interaction energy is linear in $\delta \Psi$, and, with the proper choice of the phase of $\delta \Psi$, is negative. Such modification costs kinetic and trap energy, which however is quadratic in $\delta \Psi$ for infinitesimal modification. Thus the state $\Psi^0$ for a uniform array of vortices is always unstable towards smoothing out of the density distribution. The resulting change in the density profile can be
large even though the distortions of the lattice are small.

We consider the properties of a rotating cloud in a harmonic transverse potential \( V(r) = m\omega^2_\perp (x^2 + y^2)/2 \). For simplicity, we treat mainly the two-dimensional problem, and generally set \( \hbar = 1 \). The approach adopted in Ref. [4] was to express quantities as sums over Wigner-Seitz cells for single vortices. This is cumbersome, and in this Letter we adopt a different trial condensate wave function which is better suited for rotational angular velocities close to \( \omega_\perp \).

\[
\Psi(r) = N^{1/2} h(r) \phi_{LLL} \equiv N^{1/2} \psi(r) .
\]  

The function \( h \), which we assume to be real and slowly varying on the scale of the intervortex separation, modifies the LLL components, as well as admixes higher Landau levels. The vortex lattice need not be uniform. The wave function (3) is much more convenient for calculating the kinetic energy than is the ansatz used in Ref. [4].

The admixture \( b_{\mu\nu} \) of the higher Landau level (\( \mu, \nu \)) in the wave function (3), where \( \mu \) is the angular momentum index and \( \nu \) the level index, is of order \( d^\mu_\perp (d^\nu h/dr^\perp) r^\nu_\mu \sim (d^\perp_\perp / r^\perp) (h(0) - 1) C^0_\mu \), where \( C^0_\mu \) is the amplitude of the level \( \mu \) in \( \phi_{LLL} \), and \( r^\perp_\mu = d^\perp_\perp/\hbar \) is the peak of the LLL wave function \( \mu \). The amplitude for admixture of higher Landau levels is thus of order \( d^\perp_\perp / R \sim 1/N^1_\perp \), relative to the modification of the LLL contribution, where \( N^1_\perp \) is the total number of vortices in the cloud.

The energy per particle of the condensate in the rotating frame is \( E' = E - \Omega L_z \), where \( E \) is the energy in the non-rotating frame and \( L_z \) is the expectation value of the angular momentum per particle about the rotation axis. Following Ho [1], we write

\[
E' = (\omega_\perp - \Omega) L_z + \int d^2r \ |\nabla \times \mathbf{r}| \left( \frac{m}{im} - \omega_\perp \times \mathbf{r} \right)^2 + \frac{g_{2D}}{2} |\psi|^2 \psi ,
\]

(4)

where \( \omega_\perp = \omega_\perp \hat{z} \), and \( g_{2D} \) is the effective coupling parameter in two dimensions. If the system is uniform in the \( z \) direction, \( g_{2D} = N g / Z \), where \( Z \) is the axial extent of the cloud, while if the system in the \( z \) direction is in the ground state of a particle in a harmonic potential of frequency \( \omega_\perp \), then \( g_{2D} = N g / d_z \sqrt{2\pi} \), where \( d_z \equiv (h/m\omega_\perp)^{1/2} \).

Because the higher Landau levels in the variational wave function (3) have probability \( \sim 1/N^1_\perp \), the angular momentum per particle is

\[
L_z = \int d^2r \frac{d^2}{d^2_\perp} \hbar^2 |\phi_{LLL}|^2 - 1,
\]

(5)

which we neglect. Furthermore, since \( h \) varies slowly in space, we shall use the averaged vortex approximation as in [4] to write [11]

\[
E' \simeq \Omega + \int d^2r (|\phi_{LLL}|^2) \left\{ \frac{1}{2m} \left( \frac{dh}{dr} \right)^2 + (\omega_\perp - \Omega) \frac{r^2_\perp}{d^2_\perp} \hbar^2 + \frac{b_{2D}}{2} \left( |\phi_{LLL}|^2 \right)^2 \right\} .
\]

(6)

Here \( b \equiv \langle |\phi_{LLL}|^4 \rangle / \langle |\phi_{LLL}|^2 \rangle^2 \simeq 1.158 \) describes the renormalization of the effective interaction due to the rapid density variations on the scale of the vortex separation [4 3 12].

**Uniform lattice.** We begin with the ansatz (3) for a uniform vortex density. The first term in brackets in Eq. (6), the extra kinetic energy due to admixture of excited Landau levels, scales as \( 1/R^2 \), as does the interaction energy. If \( g_{2D} \ll \hbar^2 / m \), the first term suppresses spatial variations of \( h \), and \( h \approx 1 \), i.e., the density profile is Gaussian. This condition is simply that \( N a_\perp / Z \ll 1 \); \( Z \) is the effective size in the \( z \) direction, bounded below by \( d_z \). In the opposite limit, \( g_{2D} \gg \hbar^2 / m \), the extra kinetic energy is unimportant, and the optimal density profile is obtained by minimizing the second and third terms in the integrand, which results in a TF density profile, in agreement with the considerations of Ref. [4].

To obtain illustrative results we employ a variational trial function that interpolates between the Gaussian and TF (G-TF) forms; exploiting the fact that \( \lim_{a \to \infty} (1 - t/a)^a = e^{-t} \), as in [13], we take

\[
h(r) = A_h \left( 1 - \frac{r^2}{\alpha L^2} \right)^{\alpha/2} e^{r^2/2\sigma^2} ,
\]

(7)

for \( 0 \leq r < \sqrt{\alpha L} \), and \( h = 0 \) otherwise. Expression (4) describes both the Gaussian (\( \alpha \to \infty \)) and TF (\( \alpha = 1 \)) regimes. The number of particles per unit area is \( \sqrt{\hbar^2/|\phi_{LLL}|^2} \); thus \( A^2_h = (\sigma^2 / L^2)(1 + 1/\alpha) \). We refer to Eq. (7) for \( h \) as the G-TF form.

Substituting Eq. (7) into (6), we obtain

\[
E'_{G-TF} = \Omega + \frac{\omega_\perp}{2} d^1_\perp \left\{ \frac{1}{L^2} \left[ \frac{\alpha + 1}{\alpha - 1} - \frac{2}{\sigma^2} + \frac{\alpha - 2 \sigma^4}{\alpha + 2 \sigma^4} \right] \right\} + \left( \omega_\perp - \Omega \right) \frac{\alpha}{\alpha + 2} \frac{L^2}{d^2_\perp} + \frac{b_{2D}}{2\pi} \left( \frac{\alpha + 1}{\alpha(2a + 1)} \right)^2 .
\]

(8)

Minimization of \( E'_{G-TF} \) with respect to \( \sigma \) and \( L \) yields

\[
L^2 = d^2_\perp \left( \frac{1 - \Omega}{\omega_\perp} \right)^{-\frac{1}{2}} \times \left[ \frac{1}{\alpha} \left( \alpha + 2 \right) \left\{ \frac{1}{\alpha - 1} + \kappa \left( \frac{\alpha + 1}{2a + 1} \right)^2 \right\} \right]^{\frac{1}{2}} ,
\]

(9)

and

\[
\sigma^2 = L^2 / (1 + 2/\alpha) ,
\]

(10)

where the dimensionless parameter \( \kappa = mb_{2D} / (2\pi \hbar^2) \) determines the strength of interparticle interactions.

The optimal value of \( \alpha \), determined by minimizing \( E'_{G-TF} \) with respect to \( \alpha \), obeys the quartic equation,
\[ \alpha^4 - 2(1 + 4\lambda)\alpha^3 - 12\lambda^2 + 2(1 - 3\lambda)\alpha - 1 - \lambda = 0, \]
where \( \lambda \equiv \kappa^{-1} \). The only real and positive solution is
\[ 2\alpha = \left( 2 + 2\eta\lambda + \frac{2(1 + 2\lambda)(3\eta - 1)}{\sqrt{1 + 16\eta - 3 \cdot 2^\frac{3}{2}\eta^2}} \right)^{\frac{1}{2}} + (1 + 4\lambda) + \frac{1}{\sqrt{1 + 16\eta - 3 \cdot 2^\frac{3}{2}\eta^2}}, \]
where \( \eta = \lambda(1 + \lambda) \). We note that \( \alpha \) is independent of \( \Omega \). In the weak \((\kappa \to 0)\) and strong interaction \((\kappa \to \infty)\) limits,
\[ \alpha \simeq \frac{8}{\kappa} \quad (\kappa \ll 1), \]
\[ \alpha \simeq 1 + \frac{3}{2^\frac{3}{2}}\kappa^{-\frac{3}{2}} + \mathcal{O}(\kappa^{-\frac{5}{2}}) \quad (\kappa \gg 1), \]

The shape index \( \alpha \), Eq. (11), decreases from infinity in the absence of interaction to unity as \( \alpha \) increases from zero to infinity, and the density profile of the cloud changes from a Gaussian to an inverted parabola. Without the minimization with respect to \( \alpha \), we can describe the cloud by assuming a shape of the density profile corresponding to a given value of the shape index, in terms of which \( L \) and \( \sigma \) are given by Eqs. (9) and (10). If we let \( \alpha \to \infty \), we reproduce a Gaussian density profile as in the case without the modulating function, but with optimized width.

We now compare the results for the G-TF profile with \( \alpha \) optimized and the profile with \( \alpha \to \infty \). We write the energy for the Gaussian profile as
\[ E_G' \simeq \Omega + \sqrt{2} \omega_\perp \left( 1 - \frac{\Omega}{\omega_\perp} \right)^{\frac{1}{2}} \kappa^{\frac{1}{2}}, \]

obtained by taking \( \alpha \to \infty \) in Eq. (8). The relative energy difference \((E_{G,TF}' - E_G')/(E'_G - \Omega)\) between the G-TF and Gaussian cases is shown in Fig. 1. In the limit \( \kappa \to \infty \), the energy is the TF result,
\[ E_{TF}' \simeq \Omega + \frac{4}{3} \omega_\perp \left( 1 - \frac{\Omega}{\omega_\perp} \right)^{\frac{1}{2}} \kappa^{\frac{1}{2}}, \]

and \((E_{G,TF}' - E_G')/(E'_G - \Omega)\) converges to \((2^{3/2}/3) - 1 \approx -0.0572\), independent of \( \Omega \) (Fig. 1).

In the experiments in Ref. 2, where \( \omega_z = 2\pi \times 5.3 \) Hz, \( N = 1.5 \times 10^9 \), and \( a_z = 5.6 \) nm for the triplet state of \(^{87}\text{Rb}\), one has \( N a_z / Z \gtrsim 26 \) at \( \Omega = 0.989 \omega_\perp \), typical of the highest angular velocities achieved so far. For a uniform density in the axial direction, with \( g_{2D} = gN/Z \), we find \( \kappa = 2Na_z b / Z \gtrsim 52 \), while for a Gaussian density profile in \( z \), for which \( g_{2D} = gN / d_z \sqrt{2\pi} \), we obtain \( \kappa = 2Na_z b / d_z \sqrt{2\pi} \approx 1.4 \times 10^2 \).

In Fig. 2 we plot the normalized density profile \( \nu(r) = h^2 \langle |\phi_{LLL}(Z)|^2 \rangle \) at \( \Omega = 0.99 \omega_\perp \) and \( \kappa = 100 \) for the G-TF case in addition to \( \nu(r) \) for the two extreme cases of the Gaussian form with \( \alpha \to \infty \) and the inverted TF parabola; see below. The density profile for the G-TF modulation (dashed line) is closer to the TF form than to a Gaussian. Figure 1 indicates that the relative energy reduction compared with \( E - \Omega \) for the Gaussian approximation is only \( \approx 4.95\% \).

**Distorted lattice.** Next we consider an LLL wave function with a non-uniform vortex density, and take \( h(r) = 1 \). Equation (3) is still valid, and the energy, given by
\[ E' = \Omega + \int d^2r \left( \omega_\perp - \Omega \right) r^2 \langle |\phi_{LLL}(Z)|^2 \rangle + \frac{bg_{2D}}{2} \left( \langle |\phi_{LLL}(Z)|^2 \rangle \right)^2, \]
is minimized by the TF profile
\[ \langle |\phi_{LLL}(Z)|^2 \rangle = \frac{1}{bg_{2D}} \left( \mu - \Omega - \omega_\perp \right) r^2 \],
where \( \mu \) is the chemical potential. Such a solution is possible only if one relaxes the constraint of a regular lattice; otherwise the solution is a Gaussian, as in [1].
The energy is given by the TF result \[15\]. Since the term in Eq. \[16\] involving \(dh/dr\) is positive definite, it is clear that it is energetically favorable to create deviations of the density profile from \(\phi^2_{\text{LLL}}\) by deforming the lattice rather than by exciting higher Landau levels. These conclusions have recently been confirmed by numerical calculations by Cooper et al. \[14\]. Excitation of higher Landau levels will reduce the energy of a distorted lattice still further, but it may be shown that this is of order \((gn)^2/h\Omega\) per particle, which is smaller than the terms we have retained.

Remarkably, the energy and TF profile are valid for all interactions strong enough that the averaged vortex approximation is valid. This holds provided the size of the cloud is large compared with \(d_1\), or alternatively that the number of vortices in the cloud \(N_v\approx R^2/d_1^2\) is large compared with unity. This condition is equivalent to \(NaN_s/Z\gg\Omega/\omega_1\), i.e., that the energy, \(h(\omega_1-\Omega)\), to excite higher angular momenta \(\mu\) in the LLL, be small compared with the mean field energy in the situation that all particles are in the transverse ground state of the trap. For \(\Omega\) close to \(\omega_1\), this condition for a TF profile is much weaker than that for a non-rotating cloud. By contrast, a TF profile with a uniform lattice requires \(NaN_s/Z\gg1\).

Modifying the amplitudes of lowest Landau level components in the condensate wave function, without introducing excited Landau level components, is equivalent to changing the positions of the vortices. In the LLL wave function \[11\], the positions of vortices determine the smoothed density distribution generally through \[11\],

\[
\frac{1}{4} \nabla^2 \ln n(r) = - \frac{1}{d_1^2} + \pi n_s(r).
\]

This equation allows us to estimate the displacement of the vortices from a triangular lattice for a general density distribution. In particular, if we assume a TF distribution, \(n(r)\approx 1-r^2/R^2\), where \(R\) is the radial extent of the cloud, then Eq. \[15\] implies

\[
n_v(r) = \frac{1}{\pi d_1^2} - \frac{1}{\pi R^2} \frac{1}{(1-r^2/R^2)^2}.
\]

The second term is of order \(1/N_v\) compared with the first, since \(N_v\approx R^2/d_1^2\). The corresponding mean displacement \(\delta r\) in the radial direction of the vortices at radius \(r\) is then \(\delta r/r = (d_1^2/2R^2)/(1-r^2/R^2)\approx 1/N_v\).

Thus in the LLL limit very small distortions of the lattice can result in large changes in the density distribution. For lower rotation rates, Sheehy and Radzihovsky \[16\] have recently demonstrated that the vortex density obeys an equation of the form \[16\] but with a coefficient of the second term which depends on the ratio of the vortex separation to the vortex core size. Such distortions of the vortex lattice have been measured experimentally at relatively low rotation rates \[15\], and are in good agreement with theory \[16\]. It would be valuable to extend the measurements to rapidly rotating condensates.

We thank Nick Read for stimulating correspondence, and V. Cheianov, Nigel Cooper and James Anglin for helpful comments. Author GW thanks K. Sato, K. Yasuoka, and T. Ebisuzaki for encouragement and L. M. Jensen, and P. Urkedal for help with computer facilities. Author GB thanks the Japan Society for the Promotion of Science and T. Hatsuda for enabling him to spend a fruitful research period at the University of Tokyo. This work was supported in part by Grants-in-Aid for Scientific Research provided by the Ministry of Education, Culture, Sports, Science and Technology through Research Grant No. 14-7939, by the Nishina Memorial Foundation, and by NSF Grant PHY00-98353.

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