Vortex in a trapped Bose-Einstein condensate with dipole-dipole interactions

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We calculate the critical rotation frequency at which a vortex state becomes energetically favorable over the vortex-free ground state in a harmonically trapped Bose-Einstein condensate whose atoms have dipole-dipole interactions as well as the usual s-wave contact interactions. In the Thomas-Fermi (hydrodynamic) regime, dipolar condensates in oblate cylindrical traps (with the dipoles aligned along the axis of symmetry of the trap) tend to have lower critical rotation frequencies than their purely s-wave contact interaction counterparts. The converse is true for dipolar condensates in prolate traps. Quadrupole excitations and centre of mass motion are also briefly discussed as possible competing mechanisms to a vortex as means by which superfluids with partially attractive interactions might carry angular momentum.

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I. INTRODUCTION

The achievement of Bose-Einstein condensation (BEC) in a trapped gas of \(^{52}\)Cr atoms by the Stuttgart group \(^1\) is the first instance of a condensate with large dipole-dipole interactions. In comparison to alkali atoms, which have a maximum magnetic dipole moment of \(\mu = 1\mu_B\) (\(\mu_B\) is the Bohr magneton), chromium atoms possess an anomalously large magnetic dipole moment of \(\mu = 6\mu_B\). The long-range part of the interaction between two dipoles separated by \(\mathbf{r}\), and aligned by an external field along a unit vector \(\hat{\mathbf{e}}\) (in this paper we shall always assume the dipoles are aligned by an external field), is given by

\[ U_{dd}(\mathbf{r}) = \frac{C_{dd}}{4\pi} \epsilon_{ij} \epsilon_{kl} \frac{(\delta_{ij} - 3\hat{\mathbf{r}}_i \hat{\mathbf{r}}_j)}{r^3} \]  (1)

where the coupling \(C_{dd} = \mu_0 \mu^2\) depends on the square of the dipole moment. Chromium atoms also have shorter range isotropic interactions which are asymptotically of the van der Waals-type and so fall off as \(r^{-6}\). At ultralow temperatures the de Broglie wavelength of the atoms is much larger than the range of the isotropic interactions which can consequently be handled within perturbation theory by using the usual delta-function pseudo-potential \(^2\)

\[ U(\mathbf{r}) = 4\pi \hbar^2 a_s \delta(\mathbf{r})/m \equiv g \delta(\mathbf{r}) \]  (2)

characterized solely by the s-wave scattering length \(a_s\). A measure of the strength of the long-range dipole-dipole interaction relative to the s-wave scattering energy is given by the dimensionless quantity

\[ \epsilon_{dd} \equiv \frac{C_{dd}}{3g}. \]  (3)

For \(^{87}\)Rb one finds \(\epsilon_{dd} \approx 0.007\), and Na has \(\epsilon_{dd} \approx 0.004\). Taking the s-wave scattering length of \(^{52}\)Cr to be \(a_s = 105a_B\) \(^1\), one obtains \(\epsilon_{dd} \approx 0.144\). In a further significant development, the Stuttgart group has also studied Feshbach scattering resonances between \(^{52}\)Cr atoms \(^3\). This means that the magnitude and sign of \(\epsilon_{dd}\), and thus also the value of \(\epsilon_{dd}\), can be controlled.

The principal effect of the anisotropy of the dipole-dipole interactions upon a stationary, trapped, condensate will be to distort its aspect ratio so that it is elongated along the direction of the external field \(^4\)\(^5\). This is in contrast to the case of purely isotropic interactions, for which the aspect ratio of the condensate matches that of the trap. By adopting an elongated aspect ratio along the direction of polarization, the condensate achieves a lower energy by placing more dipoles end-to-end in which configuration they are attractive, and reducing the number of repulsive side-by-side interactions. When \(\epsilon_{dd}\) exceeds a certain value, which in general depends on the aspect ratio the trap as well as the total number of atoms \(N\), mean-field theory predicts that the condensate becomes unstable to collapse \(^4\)\(^5\)\(^6\)\(^7\)\(^8\). The partially attractive nature of the dipole-dipole interaction is also responsible for introducing a curious ‘roton’ minimum \(^3\)\(^9\)\(^10\) into the Bogoliubov excitation spectrum of a uniform dipolar BEC, reminiscent of that found in the excitation spectrum of liquid helium II. It is possible that this roton minimum is indicative of an instability towards the formation of a density wave \(^11\)\(^12\).

The fact that the interaction between dipoles aligned by an external field along the axis of symmetry of a cylindrical trap are on average repulsive in an oblate (pancake shaped) BEC, but, conversely, are on average attractive in a prolate (cigar shaped) BEC, means that the sign of the dipolar mean-field energy can be controlled via the aspect ratio of the trap. In this paper we are interested in calculating the effect that this change of aspect ratio of the trap has upon the vortex state in a trapped dipolar BEC. The case of a vortex in a trapped BEC with repulsive short-range interactions, as described by Eq. (2) with \(a_s > 0\), has been extensively studied both
Theoretical, e.g. [13, 14, 15], and experimentally, e.g. [16, 17, 18]. Attractive short-range interactions have, on the other hand, received comparatively less attention, although a rotating BEC with attractive interactions is of considerable fundamental interest [19]. In particular, when the interactions are attractive it is intuitively plausible that vortex formation will be suppressed because it is energetically expensive to form the vortex core since this requires moving atoms from the centre of the BEC where they interact with many other atoms and placing them on the edges where the interact with fewer [20]. Instead, it has been proposed that the angular momentum might be preferentially absorbed into other types of excitation, such as centre of mass motion or shape oscillations, which cause much less disturbance to the condensate density profile and internal correlations [14, 21]. We also note that a recent theoretical study of a two-dimensional BEC with purely attractive short-range interactions found a new class of vortices in the form of bright ring solitons [22]. When it comes to dipolar interactions, which are partly attractive, partly repulsive, one might therefore anticipate rotational properties similar to those of standard BECs with either attractive or repulsive interactions, depending upon whether the dipolar BEC is prolate or oblate, respectively.

The latest experiments on chromium [23] have detected the first evidence of dipolar interactions upon the dynamics of a BEC by observing the ballistic expansion of the BEC when the trap is switched off. The results are in good agreement with theoretical predictions [24] giving us some confidence in the theory of dipolar BECs which has been built up over the last six years. In the following we will discuss a vortex in a rotating dipolar BEC in the Thomas-Fermi (hydrodynamic) regime, which is defined as being when the quantum zero-point kinetic energy due to the confinement by the trap is negligible in comparison to the trapping and interaction energies. This is the relevant regime when there are a large number of atoms. We shall make extensive use of the exact results for dipolar BECs in the Thomas-Fermi limit reported in references [25] and [26]. The key insight of those papers was that the dipolar mean-field potential that the atomic dipoles feel, and which is non-local, i.e. depends on the entire atom distribution, can be expressed in terms of derivatives of a scalar potential that is a solution of the Poisson equation with the dipolar density as a source. In other words, this scalar potential is formally equivalent to the electrostatic potential one would get if the density distribution were not one of dipoles but of charges, and thus standard mathematical techniques known from electrostatics can be applied. Three recent theory papers [27, 28, 29] have dealt with the structure of vortex lattices in dipolar BECs, but our aim here is to investigate the differences between dipolar and non-dipolar condensates in the case of a single vortex. Our main concern will be the calculation of the critical rotation frequency $\Omega_c$ necessary to make a single vortex energetically favorable over the ground state. Note that reference [29] also deals with the single vortex case, but their focus was somewhat different. One of their principle results was that in the case of dipolar interactions plus attractive contact interactions (negative scattering length) the vortices develop a 'craterlike' structure which is probably connected with the density wave instability mentioned above. We shall come back to this point in Section III however we shall not explicitly consider negative scattering lengths here because we wish to use some exact results that only hold in the Thomas-Fermi limit. A dipolar BEC with attractive short-range interactions is unstable to collapse in the Thomas-Fermi limit and so we limit ourselves to $a_s > 0$.

II. ENERGY FUNCTIONAL FOR A DIPOlar BEC WITH A VORTEX

Consider a condensate at $T = 0$ with a wave function $\Psi(r)$ normalized to the total number of atoms $\int |\Psi(r)|^2 d^3r = N$. The general form of $\Psi(r)$ when there is one singly quantized vortex present can be expressed in cylindrical coordinates $(\rho, \phi, z)$ as $\Psi(r) = |\Psi(\rho, z)| \exp i \phi$. This state carries an angular momentum $L_z = Nh$. In a frame rotating at angular velocity $\Omega$ about the z-axis the energy of the condensate becomes $E' = E - \Omega L_z$, where the angular momentum $L_z$ and energy $E$ are those pertaining to the laboratory frame. However, creating a vortex costs energy. Denoting the energy of the BEC in its ground state without any vortex ($L_z = 0$) by $E_0$ and the extra energy needed to make a single vortex by $E_v$, we can write the energy of the vortex state in the rotating frame as

$$E' = E_0 + E_v - \Omega L_z .$$

Thus we see that for a BEC at equilibrium in a trap rotating at angular velocity $\Omega$ the vortex state becomes energetically favorable when $\Omega$ exceeds a critical rotational velocity

$$\Omega_c = \frac{E_v}{Nh}. \quad (5)$$

To obtain $\Omega_c$ we thus need to evaluate the extra energy associated with the formation of the vortex. The total energy functional for a trapped dipolar BEC can be written as

$$E_{\text{tot}} = E_{\text{kinetic}} + E_{\text{trap}} + E_{\text{aw}} + E_{\text{dd}} \quad (6)$$

where, in terms of the condensate wave function $\Psi(r)$,

$$E_{\text{kinetic}} = -\frac{\hbar^2}{2m} \int d^3r \nabla^2 \Psi^*(r) \nabla^2 \Psi(r) \quad (7)$$

is the kinetic energy, and

$$E_{\text{trap}} = \frac{m}{2} \frac{v_s^2}{\hbar^2} \int d^3r |\Psi(r)|^2 \left[ \rho^2 + \gamma^2 z^2 \right] \quad (8)$$
is the energy due to the harmonic trap $V_{\text{trap}} = (m/2)\omega^2_x r^2 + \gamma r^2$, where $\gamma = \omega_x^2 + \gamma^2 z^2$.

\[
\gamma \equiv \omega_z / \omega_x
\]  

(9)

is the ratio of the trap frequencies. Note that in this paper we shall assume that both the trap and the condensate are cylindrically symmetric about the $\hat{z}$ direction, so in particular $\omega_x = \omega_y$, and the external field responsible for aligning the dipoles is along the $\hat{z}$ axis.

The total mean-field interaction energy can to a good approximation be written as the sum of two parts. The first is due to the isotropic short-range interactions which give rise to pure $s$-wave scattering

\[
E_{\text{sw}} = \frac{g}{2} \int d^3 r |\Psi(r)|^4
\]  

(10)

and the second is due to dipole-dipole interactions

\[
E_{\text{dd}} = \frac{1}{2} \int d^3 r d^3 r' |\Psi(r)|^2 U_{\text{dd}}(r-r') |\Psi(r')|^2.
\]  

(11)

The long-range and anisotropic nature of the dipole-dipole interaction, $U_{\text{dd}}(r)$, makes the calculation of $E_{\text{dd}}$ a non-trivial exercise. However, in the Thomas-Fermi regime some exact results (within mean-field theory) are available. In particular, an exact solution of the vortex-free Thomas-Fermi problem for a dipolar BEC in a harmonic trap yields a density profile which is an inverted parabola \[25\] \[26\]. This solution is similar to the familiar non-dipolar case \[2\], except that the aspect ratio of the cloud in the dipolar case is no longer identical to that of the trap but is stretched along the direction of the polarizing field, as mentioned above. By applying scaling transformations to this exact solution one can also describe the lowest energy collective excitations of the condensate \[25\], as well as the expansion dynamics when the trap is turned off. In the Thomas-Fermi regime the critical ratio of the dipolar and $s$-wave interactions above which instabilities occur is $\varepsilon_{\text{dd}} = 1 \[30\]$. The occurrence of these instabilities is indicated by the appearance of imaginary frequencies for the collective excitations. Another particularly novel instability in a trapped dipolar BEC, which originates from the long-range nature of the interatomic interactions, is the appearance of a local minimum in the mean-field potential outside the condensate when $\varepsilon_{\text{dd}} > 1$. This stimulates the formation of a ‘Saturn-ring’ around the condensate as atoms tunnel into the minimum \[20\].

As explained at length in references \[25\] and \[26\], the dipole-dipole interaction can be re-expressed so as to take advantage of the large technical machinery that exists to deal with electrostatic interactions. In general one can write

\[
E_{\text{dd}} = \frac{1}{2} \int d^3 r \ n(r) \Phi_{\text{dd}}(r)
\]  

(12)

where $\Phi_{\text{dd}}(r)$ is the non-local dipolar mean-field potential

\[
\Phi_{\text{dd}}(r) \equiv \int d^3 r' \ U_{\text{dd}}(r-r') n(r')
\]  

(13)

For dipoles aligned along $\hat{z}$ this dipolar mean-field potential can in turn be expressed in terms of a fictitious electrostatic potential $\phi(r)$

\[
\Phi_{\text{dd}}(r) = -C_{\text{dd}} \left( \frac{\partial^2}{\partial z^2} \phi(r) + \frac{n(r)}{3} \right)
\]  

(14)

which is obtained from the “charge” distribution $n(r)$ in the usual way

\[
\phi(r) = \frac{1}{4\pi} \int d^3 r' \frac{n(r')}{|r-r'|}
\]  

(15)

where, of course, $n(r)$ and $\phi(r)$ satisfy Poisson’s equation $\nabla^2 \phi = -n(r)$. This formulation of the problem allows us to immediately identify some generic features of dipolar gases. For example, if $n(r)$ and hence $\phi(r)$ are uniform along the polarization direction ($\hat{z}$) then the non-local part of the dipolar interaction vanishes because of the $\partial^2 / \partial z^2$ operator. A very prolate pencil-like condensate, i.e. one which has $R_x \gg R_y, R_z$ will therefore be largely unaffected by the non-local part of the interaction except perhaps at the very ends of the condensate if the density profile has a large curvature there. Thus, in the very prolate (or entirely homogenous) case the contribution of dipolar interactions to the mean-field potential reduces to that of the local term $\Phi_{\text{dd}}(r) \rightarrow -C_{\text{dd}} n(r)/3$ whose effect is then simply to modify the magnitude of the local mean-field potential arising from the pure $s$-wave interactions. A related example to a very prolate BEC is a BEC with a generic smooth outer density profile but which is, however, penetrated by a pencil-like vortex or vortices: the dipolar potential would be expected to peak around the ends of each vortex where the density profile is rapidly changing in the $z$-direction. One might conjecture that the curious ‘craterlike’ density profile around the ends of vortices in dipolar BECs that has recently been seen in simulations \[24\] is connected to this effect.

Let us consider the case of a parabolic density profile of the form

\[
n_{\text{bg}}(r) = n_0 \left( 1 - \frac{\rho^2}{R_x^2} - \frac{z^2}{R_z^2} \right)
\]  

(16)

As stated above, a parabolic density profile is an exact solution of the hydrodynamic equations for a non-rotating BEC in the Thomas-Fermi limit even in the presence of dipolar interactions. Here the subscript “bg” stands for “background”, i.e. for a condensate without a vortex but on top of which we will superimpose a vortex later on. One finds that the dipolar mean-field potential inside a condensate with the parabolic density profile \[10\] is given by \[24\] \[26\]

\[
\Phi_{\text{bg}}^{\text{dd}}(r,z) = -n_0 C_{\text{dd}} \left[ \frac{\rho^2}{R_x^2} - \frac{2z^2}{R_z^2} - f(\kappa) \left( 1 - \frac{3}{2} \frac{\rho^2 - 2z^2}{R_x^2 - R_z^2} \right) \right]
\]  

(17)

In this expression

\[
f(\kappa) = \frac{2 + \kappa^2 [4 - 3\Xi(\kappa)]}{2(1 - \kappa^2)}
\]  

(18)
is a function of $\kappa$ which is the aspect ratio of the BEC,

$$\kappa \equiv R_x/R_z$$

and monotonically decreases from its value of $f = 1$ at $\kappa = 0$, passing through zero at $\kappa = 1$, tending towards $f = -2$ as $\kappa \to \infty$. The function $\Xi(\kappa)$ upon which $f(\kappa)$ depends is itself dependent upon whether the condensate density profile is prolate, in which case

$$\Xi \equiv \frac{1}{\sqrt{1 - \kappa^2}} \ln \frac{1 + \sqrt{1 - \kappa^2}}{1 - \sqrt{1 - \kappa^2}}$$

for $\kappa < 1$ (prolate) or oblate

$$\Xi \equiv \frac{2}{\sqrt{\kappa^2 - 1}} \arctan \sqrt{\kappa^2 - 1}$$

for $\kappa > 1$ (oblate).

The value of the aspect ratio $\kappa$ is given by the solution of a transcendental equation [21, 24, 25, 26].

$$3\kappa^2 \varepsilon_{dd} \left[ \left( \frac{\gamma^2}{2} + 1 \right) \frac{f(\kappa)}{1 - \kappa^2} - 1 \right] + (\varepsilon_{dd} - 1) (\kappa^2 - \gamma^2) = 0.$$  

Note that according to Eq. (17), the dipolar mean-field potential $\Phi_{dd}(\rho, z)$ is in general saddle-shaped [23], and thus inherits the anisotropic partially attractive/partially repulsive character of the dipolar interactions. The saddle-shaped mean-field potential causes an elongation of the BEC along the polarization direction which can be viewed as type of magnetostriiction. This is illustrated for five different trap aspect ratios in Fig. 1. The total energy ($E_{\text{trap}} + E_{\text{sw}} + E_{\text{dd}}$) associated with the vortex-free Thomas-Fermi solution (10) can be calculated to be

$$E_0 = \frac{N}{14} m \omega_z^2 R_z^2 \left( 2 + \frac{\gamma^2}{\kappa^2} \right) + \frac{15}{2\pi} \frac{N^2 g}{\bar{R}^2 z} \left[ 1 - \varepsilon_{dd} f(\kappa) \right].$$

The quantity $E_0$ is the ground state energy referred in Eq. (11).

Having now summarized what is already known concerning the mean-field potential inside a non-rotating dipolar BEC, let us turn to the form of the density profile of a rotating BEC with a vortex. We shall adopt the following variational ansatz for the density profile of an $N$-atom condensate with a single vortex

$$n(\mathbf{r}) \equiv |\Psi(\mathbf{r})|^2$$

$$= n_0 \left( 1 - \frac{\rho^2}{R_x^2} \right) \left( 1 - \frac{\beta^2}{\rho^2 + \beta^2} \right)$$

$$= n_{bg}(\mathbf{r}) + n_v(\mathbf{r})$$

where we have observed that the ansatz can be written as the sum of two terms: the background Thomas-Fermi parabolic profile $n_{bg}(\mathbf{r})$ as already given in Equation (10) and the vortex profile $n_v(\mathbf{r})$

$$n_v(\mathbf{r}) = -n_0 \frac{\beta^2}{\rho^2 + \beta^2} \left( 1 - \frac{\rho^2}{R_x^2} \right) \left( 1 - \frac{\beta^2}{\rho^2 + \beta^2} \right).$$

Ansatz (24) assumes that the vortex, whose core size is parameterized by $\beta$, is superimposed on a background parabolic density profile with radii $R_x = R_y$ and $R_z$. Note that the variational ansatz (24) has the correct $\rho^2$ dependence of the density as $\rho \to 0$ (with $\ell = 1$), which it must have in order to satisfy the Gross-Pitaevskii equation for a vortex of $\ell$ circulation quanta [21]. It has also got the correct asymptotic form (in terms of even powers of $1/\rho$) that the solution must have for $\rho \to \infty$. The central density $n_0$ is fixed by normalization to be

$$n_0 = \frac{15N}{8\pi R_x R_z} \left( 1 + \frac{20}{3} \beta^2 + 5\beta^4 \right)$$

$$-5\beta^2 (1 + \beta^2)^{3/2} \arctanh[1/\sqrt{1 + \beta^2}]$$

where

$$\tilde{\beta} \equiv \beta/R_x$$

is the ratio of the vortex core size to the transverse radius of the BEC.

We proceed by minimizing $E_{\text{tot}}$ as a function of the three variational parameters $R_x$, $R_z$ and $\beta$. The terms $E_{\text{kinetic}}, E_{\text{trap}}$ and $E_{\text{sw}}$ can all be calculated analytically in a straightforward albeit laborious manner. The results are presented in Appendix A. To evaluate the dipole-dipole energy functional we begin from Equation (11).
and substitute in the density ansatz \(25\)

\[
E_{dd} = \frac{1}{2} \int d^3r \ d^3r' \ n_{bg}(r)U_{dd}(r-r')n_{bg}(r')
+ \frac{1}{2} \int d^3r \ d^3r' \ n_{bg}(r)U_{dd}(r-r')n_{bg}(r')
+ \frac{1}{2} \int d^3r \ d^3r' \ n_{v}(r)U_{dd}(r-r')n_{v}(r')
+ \frac{1}{2} \int d^3r \ d^3r' \ n_{v}(r)U_{dd}(r-r')n_{v}(r').
\]

Noting that the two cross terms between the vortex and background densities are identical, i.e. the integral is invariant under exchange of the coordinates \(r\) and \(r'\), the dipolar energy functional can be written

\[
E_{dd} = \frac{1}{2} \int d^3r \ d^3r' \ n_{bg}(r)U_{dd}(r-r')n_{bg}(r')
+ \int d^3r \ d^3r' \ n_{v}(r)U_{dd}(r-r')n_{bg}(r')
+ \frac{1}{2} \int d^3r \ d^3r' \ n_{v}(r)U_{dd}(r-r')n_{v}(r').
\]

We shall now restrict ourselves to situations where the size of the vortex core is much smaller than the radius of the condensate, i.e. \(\beta \ll 1\). This is consistent with the spirit of the Thomas-Fermi approximation for the background parabolic envelope, and should hold for condensates containing a large number of atoms, providing the system does not become very prolate. To this end we shall drop the vortex-vortex part of the dipolar energy functional since this has an extra factor of \(\beta^2\) in comparison to the cross term. The remaining two terms can be expressed as

\[
E_{dd} \approx \frac{1}{2} \int d^3r \ d^3r' \ n_{bg}(r)U_{dd}(r-r')n_{bg}(r')
+ \int d^3r \ d^3r' \ n_{v}(r)U_{dd}(r-r')n_{bg}(r')
= \frac{1}{2} \int d^3r \ n_{bg}(r)\Phi_{dd}^{bg}(r) + \int d^3r \ n_{v}(r)\Phi_{dd}^{bg}(r).
\]

The first term is just the dipolar energy of the condensate without a vortex, whilst the second gives the dipolar ‘interaction’ between the vortex and the background density profile. Both terms have been reduced to single integrals of their respective density profiles over the known quadratic function \(\Phi_{dd}^{bg}(\rho, z)\), as given by Equation \(17\), which is the mean-field potential due to the background inverted parabola density profile. These integrals can therefore be evaluated relatively easily and the results are given in the Appendix.

### III. RESULTS OF MINIMIZATION OF THE ENERGY FUNCTIONAL

#### A. Oblate trap

To illustrate the oblate case we shall consider 150,000 \(^{52}\)Cr atoms in a trap having frequencies \(\omega_x = \omega_y = 2\pi \times 200 \text{ rad/s}, \omega_z = 2\pi \times 1000 \text{ rad/s}\), so that \(\gamma = 5\). The harmonic oscillator length of the trap along the \(x\)-direction is then \(a_{ho} = \sqrt{\hbar/m\omega_x} = 0.986\mu m\). We numerically minimize the total energy functional \(E_{tot}\) with respect to \(\{\beta, R_x, \kappa\}\) using the Mathematica routine \textit{NMinimize}. In order to bring out the dependence of the various quantities upon the relative strength of the two types of interactions (\(s\)-wave and dipolar) we plot the results as a function of the \(s\)-wave scattering length \(a_s\), since this quantity can be controlled in an experiment \(3\). As \(a_s \rightarrow 0\) the dipolar interactions dominate, whereas when \(a_s \rightarrow \infty\) the dipolar interactions become insignificant. The magnitude of the magnetic dipole interaction is here assumed to be fixed at the appropriate value for \(^{52}\)Cr, namely \(C_{dd} = \mu_0(6\mu_B)^2\). Note that in the case of dipoles induced by electric fields one has \(C_{dd} = E^2\alpha^2/e_0\) \(31\), where \(\alpha\) is the polarizability and \(E\) is the electric field strength, so the size of the electric dipolar interaction can be directly controlled via the magnitude of \(E\). In fact the magnitude of even magnetic dipolar interactions can be controlled independently of the \(s\)-wave interactions by rotating the magnetic field \(32\), but we presume that the experimentally easiest option is to use a Feshbach resonance to adjust \(a_s\) since only the magnitude of the magnetic field needs to be tuned.

In all the calculations depicted in the following figures we limited the minimum value of the scattering length to be \(17.5a_0\), where \(a_0\) is the Bohr radius, corresponding to \(\varepsilon_{dd} = 0.87\). This is because as \(a_s \rightarrow 0\) the approximation we made in the calculation of the energy functional that \(\beta = \beta/R_x\) be small begins to breakdown (see Figures \(4\) and \(9\)). Furthermore, in the Thomas-Fermi approximation used here collapse instabilities can occur when \(\varepsilon_{dd} > 1\). Indeed, as mentioned previously, because of these collapse instabilities one can argue that the Thomas-Fermi regime does not exist when \(\varepsilon_{dd} > 1\), see \(26\). The maximum value of scattering length was set at \(600a_0\), corresponding to \(\varepsilon_{dd} = 0.03\).

- Fig. \(2\) shows the total energy \(E_{tot}\), as defined by Eq. \(9\), of a condensate with a vortex in an oblate trap. In an oblate BEC the dipolar interactions are predominantly repulsive, which raises the energy relative to the \(s\)-wave only case.
- Fig. \(3\) plots the radial size \(R_x\) of a condensate with a vortex. In a strongly oblate BEC such as this one the majority of atoms interact via the radially repulsive part of the dipolar interaction which consequently increases \(R_x\) slightly above the pure \(s\)-wave value.
FIG. 2: Total energy (in the Thomas-Fermi approximation) of a dipolar BEC with a vortex in an oblate trap (γ = 5). Solid curve: both s-wave and dipolar interactions. Dashed curve: s-wave only. The s-wave scattering length $a_s$ is measured in units of the Bohr radius $a_0$. The energy $E_{\text{tot}}$ is measured in units of the radial harmonic trapping energy of $N$ atoms.

FIG. 3: The radial size $R_x$ of a condensate with a vortex in an oblate trap (γ = 5). Solid curve: both s-wave and dipolar interactions. Dashed curve: s-wave only. $R_x$ is measured in units of the radial harmonic oscillator length $a_{\text{ho}}$ of the trap.

• Fig. 4 shows $\bar{\beta} = \beta/R_x$, the ratio of the vortex core size to the radial size of the condensate. Note that this ratio remains small over the chosen range of parameters, which, as mentioned above, is necessary for the self-consistency of the calculation. In an oblate trap we see that the effect of the dipolar interactions is to increase $\bar{\beta}$ beyond that found in the pure s-wave case.

• Fig. 5 depicts the aspect ratio $\kappa = R_x/R_z$ of a condensate with a vortex. The magnetostriction that reduces $\kappa$ by elongating the condensate is clearly visible.

• Fig. 6 gives the critical angular velocity $\Omega_c$ of the condensate above which it is energetically favorable to form a vortex. We see that the effect of dipolar interactions in an oblate trap is to decrease $\Omega_c$.

B. Prolate trap

We now turn to the case of a prolate trap for which the dipolar interactions are predominantly attractive. We choose a trap which has the inverse aspect ratio to the previous oblate case, namely with frequencies $\omega_x = \omega_y = 2\pi \times 200$ rad/s as before, so that the harmonic oscillator length of the trap along the x-direction remains the same, but with $\omega_z = 2\pi \times 40$ rad/s, so that $\gamma = 0.2$.

• Fig. 4 depicts the total energy $E_{\text{tot}}$ of the vortex state in a prolate trap. The effect of the mainly attractive dipolar interactions is to shift the energy downwards, oppositely to the case of an oblate trap.

• Fig. 5 plots the radial size, $R_x$, of a dipolar condensate with a vortex in a prolate trap. $R_x$ is smaller than in the pure s-wave case because of the re-distribution of atoms by the anisotropic interactions.

• Fig. 6 shows that the ratio of the vortex core size to the radial size of the condensate, $\bar{\beta} = \beta/R_x$. 
FIG. 6: The critical angular velocity $\Omega_c$ above which a vortex state is energetically favorable in an oblate trap ($\gamma = 5$). Solid curve: both s-wave and dipolar interactions. Dashed curve: s-wave only. These curves were calculated using Eq. 5. $\Omega_c$ is measured in units of the radial harmonic oscillator angular frequency $\omega_x$ of the trap.

Note that this ratio remains small over the chosen range of parameters, which is necessary for the self-consistency of the calculation, although not as small as in the oblate case. Notice also that in comparison the pure s-wave case $\bar{\beta}$ is smaller in the presence of dipolar interactions in a prolate trap, and this trend is opposite to that found in an oblate trap.

• Fig. 10 gives the aspect ratio $\kappa = R_x/R_z$ of a condensate with a vortex in a prolate trap. Due to the magnetostriction $\kappa$ is smaller than in the pure s-wave case. This is the same behavior as was found in an oblate trap.

• Fig. 11 shows that, in contrast to the oblate case, the dipolar interactions in a prolate trap increase the value of the critical angular velocity $\Omega_c$ of the condensate above which it is energetically favorable to form a vortex.

IV. AN EXPLICIT EXPRESSION FOR $\Omega_c$

The effect that $\Omega_c$ is decreased in an oblate trap and increased in a prolate trap is the main result of this paper. Let us see if we can interpret this physically. The value of $\Omega_c$ shown in Figures 6 and 11 for the purely s-wave interactions (dashed curve) agrees very well with the analytic formula valid in the Thomas-Fermi limit [14]

$$\Omega_c = \frac{5}{2} \frac{\hbar}{m R_x} \ln \frac{0.67 R_x}{\xi_s}. \quad (30)$$

This is derived by integrating the kinetic energy density $n(\rho, z)v_s^2(\rho)/2$, arising from the superfluid flow $v_s = (\hbar/m)1/\rho$ around the vortex, over the profile of the condensate. The lower limit of the integral is set by the vortex core size which is given by the healing length $\xi_s$

$$\xi_s = \frac{1}{\sqrt{8\pi n_0 a_s}}. \quad (31)$$

The relevant density appearing in this expression is taken to be the density at the centre of the trap $n_0$ in the absence of a vortex, which in the Thomas-Fermi limit is given by

$$n_0 = \frac{15N}{8\pi} \frac{1}{R_x R_z}. \quad (32)$$

In the Thomas-Fermi regime the radii of a condensate with s-wave interactions obey [2]

$$R_i = a_{ho} \left( \frac{15Na_s}{a_{ho}} \right)^{1/5} \frac{\omega_{ho}}{\omega_x} \quad (33)$$

where $\omega_{ho} = (\omega_x \omega_y \omega_z)^{1/3}$ and $a_{ho} = \sqrt{\hbar/(m\omega_{ho})}$. Combining all these quantities together one finds that as $a_s \rightarrow 0$ the critical rotation frequency diverges as $\Omega_c \propto$
\[ a_s^{-2/5} \log a_s, \text{ although, of course, eventually the neglected quantum pressure term will prevent this divergence.} \]

Now consider the dipolar case. A formula for \( \Omega_c \) closely resembling (30) should still apply. Indeed, the inverted-parabola Thomas-Fermi density profile is common to both the s-wave and dipolar cases and it is this that gives rise to the specific 5/2 and 0.67 numerical factors appearing in (30). The one difference we might expect concerns the lower limit of the integration which is set by the vortex core size. In the presence of dipolar interactions we can no longer assert that the core size is solely determined by \( \xi_s \) since this makes no reference to dipolar interactions. Indeed, we might expect that as the scattering length vanishes it is replaced by an equivalent length scale set by the dipolar interactions of the form \( a_d = (C_{dd}/3)m/(4\pi\hbar^2) \). However, expression (30) only has logarithmic accuracy \[ 35\] and is relatively insensitive to the lower cutoff \( \xi_s \) of the kinetic energy integral appearing inside the logarithm. The dominant change in (30) due to the presence of dipolar interactions is therefore likely to be in the radial size \( R_x \). This makes one wonder whether the same expression (30) for \( \Omega_c \) approximately holds for dipolar BECs if the radius \( R_x \) is modified to include the effect of the dipole-dipole interactions but the changes in the healing length are ignored? The answer to this question is yes \[ 34\] as we shall now show.

The Thomas-Fermi radii of a vortex-free BEC cylindrically symmetric in the \( x - y \) plane (dipoles aligned along \( z \)) with both contact and dipolar interactions are \[ 25\, 26\]

\[ R_x = R_y = \left[ \frac{15g_N\kappa}{4\pi m\omega_x^2} \left\{ 1 + \varepsilon_{dd} \left( \frac{3\kappa^2 f(\kappa)}{2 - 1 - \kappa^2} - 1 \right) \right\} \right]^{1/5} \]

and \( R_z = R_x/\kappa \). The function \( f(\kappa) \) appearing in this expression is given by Eq. (15) and the value of \( \kappa \) is determined by the transcendental Eq. (22). In Fig. 12 we compare the value of \( \Omega_c \) calculated by the energy minimization method presented in Section III with the value of \( \Omega_c \) obtained from the explicit expression (30) where \( R_x \) is given by (34). The agreement is strikingly good, with the exception of very small \( a_s \) in the prolate case. In fact, in view of the closeness of the match one is tempted to conclude that whilst the long-range dipolar interactions strongly influence the boundary of the condensate and hence the large scales represented by \( R_x \), the shorter range van der Waals interactions which set the scale for \( a_s \) and hence \( \xi_s \) continue to dominate the shorter range physics setting the size of the vortex core, except when \( a_s \) becomes very small indeed.

V. COMPARISON OF VORTICES WITH OTHER TYPES OF ANGULAR MOTION

We have seen in previous sections that for a dipolar BEC in a rotating prolate trap, the formation of a vortex is increasingly energetically suppressed as the dipolar interactions grow in strength. Indeed, once \( \Omega_c \geq \omega_z \) the vortex would be impossible to realize, in a harmonic trap at least, because the trap can no longer counteract the centrifugal force and the BEC would fly apart (neglecting, of course, the intriguing possibility that the
by the magnitude of the interactions (but perhaps, based on the discussion of Section IV, the effect of dipolar interactions is simply through the degree to which these change the shape and aspect ratio of the condensate). One might tentatively conjecture, therefore, that as the critical rotation frequency for energetic favorability of the vortex state goes up, and the critical rotation frequency for the dynamical instability towards shape oscillations goes down, shape oscillations will be formed that will not go on to form vortices.

Let us now also briefly consider another possibility, namely oscillations of the centre of mass (CM). In a harmonic trap CM oscillations decouple from internal excitations provided the interactions are pairwise, and therefore take place at the trap frequency. Like low-lying shape oscillations, CM oscillations also preserve the parabolic density profile and so might be energetically preferable to a vortex in the presence of attractive interactions. Consider a BEC executing a CM oscillation of the form

$$ \mathbf{r}_{cm}(t) = r_0 \cos(\omega_c t) \hat{x} + r_0 \sin(\omega_c t) \hat{y} $$  \hspace{1cm} (35)$$

where $\mathbf{r}_{cm}(t)$ is the position of centre of mass of the BEC, which behaves like a classical particle of mass $Nm$ with potential energy $NM\omega_c^2 r_{cm}^2/2$. This circular motion has an angular momentum $L_{cm} = Nm\omega_c r_{cm}^2$, with the actual value of $L_{cm}$ being determined by the radius $r_0$. Note that (35) describes dynamics obeying the superfluid irrotationality condition ($\nabla \times \mathbf{u} = 0$) as may be verified by observing that the wave function which is an exact solution of the time-dependent Gross-Pitaevskii equation describing this type of motion is of the form [2]

$$ \Psi(r, t) = \exp[-i\mu t/\hbar] \exp[i\alpha(t)|x - A(t)/2|/\hbar] \times \exp[i\beta(t)|y - B(t)/2|/\hbar] \times \Psi_0(x - A(t), y - B(t), z) $$  \hspace{1cm} (36)$$

where $\Psi_0(x, y, z)$ is a stationary state satisfying the time-independent Gross-Pitaevskii equation, and the parameters $\{A(t), \alpha(t); B(t), \beta(t)\}$ obey $a = mA, Am\omega^2_c = -\alpha$ and $\beta = mB, Bm\omega^2_c = -\beta$.

The energy associated with the type of CM oscillations given by (36) is $E_{cm} = Nm\omega_c^2 r_{cm}^2/r_0^2$. In order to make a comparison between the energy of the vortex state and the CM motion we set $L_{cm} = Nh$, so that the two have the same angular momentum. Then $r_{cm}^2 = h/(m\omega_c)$, i.e. the radius of motion is equal to the trap oscillator length, and so $E_{cm} = Nh\Omega_c$. Noting that the ground state energy, $E_0$, is the same for both the vortex and CM motion, we can therefore compare $E_{cm}$ with $E_0 = Nh\Omega_c$. In order to be competitive with a vortex, CM motion with $L_{cm} = Nh$ would therefore require $\Omega_c \geq \omega_c$, but this is exactly the rotational speeds for which the harmonic trap no longer confines the atoms and so we surmise that CM motion is not energetically favorable over a vortex state in a harmonic trap. This does not preclude, however, that centre of mass motion takes place in preference to other types motion for angular momenta $L < Nh$. Also, attractive nature of the mean-field interactions might be capable of holding the condensate together for rotational frequencies $\Omega$ greater than $\omega_c$. The question then arises, how does a prolate dipolar BEC rotate? One possibility is for the condensate to generate other types of excitation that carry angular momentum, such as quadrupole shape oscillations which have an azimuthal angular momentum projection $m = 2$. In the frame of reference rotating with the trap a quadrupole oscillation appears as a stationary distortion of the density profile in the $x - y$ plane and it is generated through a dynamical instability which has a threshold frequency $\Omega_{dyn}$ that in the pure s-wave case is typically considerably higher than $\Omega_c$ (in the case of an axisymmetric trap $\Omega_{dyn} = \omega_c/\sqrt{2}$). Dynamical instabilities corresponding to shape oscillations play an important role in the dynamics of how a vortex actually enters the condensate, a subject we have not touched upon since we have only considered the energetics rather than the dynamics of vortex formation. In the case of pure s-wave condensates it is an experimental fact that in order to generate vortices the trap must be rotated at a frequency considerably exceeding the condition of energetic stability given by Eq. (39) and instead corresponding closely to $\Omega_{dyn}$.

The dynamical instability of a rotating dipolar BEC to shape oscillations has recently been investigated, and it was found that dipolar interactions always lower the threshold rotational frequency $\Omega_{dyn}$ at which the dynamical instability occurs, in both the prolate and oblate cases. It is interesting to note that in the pure s-wave case the threshold frequency for the instability is independent of interaction strength (even though the instability relies on the existence of two-body interactions) but, conversely, in the dipolar case is strongly affected

![FIG. 12: Comparison of the critical angular velocity $\Omega_c$ calculated by the methods of Section III (solid curves) with the prediction of the analytic formula Eq. (30) where the condensate radius $R_c$ is calculated for a dipolar BEC in the Thomas-Fermi limit with no vortex (dash-dot curves), see text for details. The upper two curves are for the prolate case, $\gamma = 0.2$, and the lower two curves are for the oblate case, $\gamma = 5$, as before. Note that the match is so good that it is hard to discern the difference between the solid and the dash-dot curves, except for very small $a_s$ in the prolate case.](image-url)
perhaps centre of mass motion can be favored in non-harmonic traps.

VI. CONCLUSIONS

The question of how quantum fluids rotate is a fascinating one. The versatility of atomic BECs means that this problem can now be studied in systems with repulsive or attractive interactions, as well as the case of dipole-dipole interactions which are partially repulsive partially attractive and long range. In this paper we have used an approach based on an analogy to electrostatics that allows the explicit calculation of the anisotropic mean-field potential inside a dipolar BEC. This approach gives quite general insight and in particular shows that the long-range part of the interaction is especially important in places where the density profile has a large curvature in the direction of polarization, such as the ends of vortices. Numerical minimization of the total energy functional calculated by this method in the Thomas-Fermi regime indicates that, in comparison to the case of pure $s$-wave contact interactions, dipolar interactions lower the critical rotation frequency $\Omega_c$ of a BEC necessary to make a vortex energetically favorable in an oblate harmonic trap and raise the critical rotation frequency in a prolate harmonic trap.

The same results can also be accurately reproduced using the analytic formula Eq. (30) well known in the usual case of $s$-wave contact interactions providing the modification of the radius $R_x$ of the BEC due to dipolar interactions is accounted for using Eq. (33). The analytic formula allows one to attribute the principal change in $\Omega_c$ caused by the dipolar interactions to changes in $R_x$, i.e., large scale changes in the overall shape of the condensate, rather than changes on the much smaller scale of the healing length which determines the size of the vortex core. Finally, we have also discussed angular momentum carrying shape oscillations as well as centre of mass oscillations as competitors to vortices in rotating prolate dipolar BECs, and tentatively conclude that under certain circumstances shape oscillations such as the quadrupole oscillation may be preferred.

APPENDIX A: THE ENERGY FUNCTIONALS

In this appendix we write down the explicit expressions for the functionals giving the kinetic, trapping, $s$-wave scattering, and dipolar interaction energy of the condensate, as defined by Equations (7), (8), (10), and (11), respectively. Beginning with the kinetic energy, we first note that in cylindrical coordinates the gradient is given by

$$\nabla = \hat{e}_\rho \frac{\partial}{\partial \rho} + \hat{e}_\phi \frac{\partial}{\partial \phi} + \hat{e}_z \frac{\partial}{\partial z}$$

(A1)

which acts upon the wave function given by the square root of the density ansatz $|\Psi|^2$.

$$\Psi(\rho, \phi, z) = \sqrt{n_0} \sqrt{1 - \frac{\rho^2}{R_x^2}} \sqrt{1 - \frac{\beta^2}{\rho^2 + \beta^2}} e^{i\phi}.$$  

(A2)

The phase $\phi$ accounts for the superflow around the vortex in the usual way, viz. $v_x = (\hbar/m)\nabla \phi$. However, the Thomas-Fermi approximation corresponds to neglecting the kinetic energy arising from the curvature of the slowly varying condensate background envelope $\sqrt{1 - \rho^2/R_x^2} - z^2/R_z^2$. We shall consequently drop all terms which originate from the gradient of this term. On the other hand, it is essential to retain the terms arising from the gradient of the vortex part of the wave function $\sqrt{1 - \beta^2/(\rho^2 + \beta^2)}$ which varies rapidly in the $\hat{e}_\phi$ direction, as well as the superflow term. Under these approximations we find the kinetic energy to be

$$E_{\text{kinetic}} = \frac{\hbar^2}{2m} \frac{n_0 \pi R_z}{3} \left\{ -11\beta^2 - \frac{26}{3} + \frac{11\beta^4 + 16\beta^2 + 8}{\sqrt{1 + \beta^2}} \arctanh \left[ \frac{1}{\sqrt{1 + \beta^2}} \right] \right\}$$

(A3)

where $n_0$ is the number density at the centre of the trap, as given by Equation (27).

Using the density ansatz (24) the trapping and $s$-wave scattering energies are straightforwardly evaluated to be

$$E_{\text{trap}} = \frac{2\pi}{3} n_0 m \omega_x^2 \frac{R_z^5}{\kappa} \left\{ \frac{4}{35} - \frac{2}{5} \beta^2 - \frac{8}{3} \beta^4 - 2\beta^6 
+ \frac{\omega_x^2}{5\kappa^2} \left( \frac{1}{7} + \frac{23}{15} \beta^2 + \frac{7}{3} \beta^4 + \beta^6 \right) 
+ 2\beta^2 \left[ \beta^2 - \frac{\gamma^2}{5\kappa^2} (1 + \beta^2) \right] (1 + \beta^2)^{3/2} \right\} \arctanh \left[ \frac{1}{\sqrt{1 + \beta^2}} \right]$$

(A4)
and
\[ E_{sw} = \frac{8\pi}{15} n_{bg}^2 \frac{R_x^2}{\kappa} \left[ \frac{2}{7} + \frac{107}{15} \beta^2 + 16 \beta^4 + 9 \beta^6 \right] \]
\[-\beta^2 (4 + 13 \beta^2 + 9 \beta^4) \sqrt{1 + \beta^2} \times \text{arctanh} \left( \frac{1}{\sqrt{1 + \beta^2}} \right) . \]  \hfill (A5)

The dipolar energy functional is more difficult to calculate since the dipolar mean-field potential \( \Phi_{dd}(\mathbf{r}) \) is non-local. In the text we argued that
\[ E_{dd} \approx \frac{1}{2} \int d^3r \, n_{bg}(\mathbf{r}) \Phi_{dd}(\mathbf{r}) + \int d^3r \, n_{v}(\mathbf{r}) \Phi_{dd}(\mathbf{r}) \]  \hfill (A6)

and
\[ \int d^3r \, n_{v}(\mathbf{r}) \Phi_{dd}^{bg}(\mathbf{r}) = -\frac{4\pi}{15} n_{bg}^2 \varepsilon_{dd} \frac{R_x^3}{\kappa} \left[ \frac{122}{15} + \frac{68}{3} \beta^2 + 14 \beta^4 \right] \]
\[ \frac{f(\kappa)}{15(\kappa^2 - 1)} \left[ -62 + 245 \kappa^2 + 30 \beta^2 (2 + 15 \kappa^2) + 45 \beta^4 (2 + 5 \kappa^2) \right] \]
\[-(1 + \beta^2)^{3/2} \text{arctanh} \left( \frac{1}{\sqrt{1 + \beta^2}} \right) \left[ 4 + 14 \beta^2 + \frac{f(\kappa)}{\kappa^2 - 1} (-4 + 10 \kappa^2 + 6 \beta^2 + 15 \kappa^2 \beta^2) \right] . \]  \hfill (A8)

where \( \Phi_{dd}^{bg}(\mathbf{r}) \) is given by the quadratic function Equation (17). These two integrals can be evaluated explicitly and the results are
\[ \frac{1}{2} \int d^3r \, n_{bg}(\mathbf{r}) \Phi_{dd}(\mathbf{r})^{bg} = -\frac{16\pi g n_{bg}^2}{105 \kappa} \varepsilon_{dd} R_x^3 f(\kappa) \]  \hfill (A7)

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This is most easily seen by comparing the Fourier transform of the dipolar interaction, i.e. $\tilde{U}_{dd}(k) = C_{dd} \hat{e}_i \hat{e}_j (3 \hat{k}_i \hat{k}_j - \delta_{ij})$, with that of the contact interaction, i.e. $\tilde{U}(k) = g$. One immediately sees that $\varepsilon_{dd} = 1$ corresponds to the case when the isotropic term in the dipole-dipole interaction is exactly equal and opposite to the contact interaction.

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