Dipolar Bose-Einstein condensate in a ring or in a shell

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We study properties of a trapped dipolar Bose-Einstein condensate (BEC) in a circular ring or a spherical shell using the mean-field Gross-Pitaevskii equation. In the case of the ring-shaped trap we consider different orientations of the ring with respect to the polarization direction of the dipoles. In the presence of long-range anisotropic dipolar and short-range contact interactions, the anisotropic density distribution of the dipolar BEC in both traps is discussed in detail. The stability condition of the dipolar BEC in both traps is illustrated in a phase plot of dipolar and contact interactions. We also study and discuss the properties of a vortex dipolar BEC in these traps.

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I. INTRODUCTION

After the experimental realization of dilute trapped Bose-Einstein condensate (BEC) of alkali-metal atoms [1], it was realized that for attractive atomic contact interaction the BEC is stable for the atomic interaction (measured by the scattering length) and number of atoms below a certain limit depending on the trap [1–3]. In the case of $^7$Li atoms with attractive atomic interaction, in the harmonic trap used in the experiment [2], the condensate was stable for less than about 1400 atoms. For repulsive contact interaction, the trapped BEC is unconditionally stable for all values of scattering length and number of atoms [1].

More recently, there has been experimental observation of BECs of $^{52}$Cr [4,5], $^{164}$Dy [6,7], and $^{168}$Er [8] with large long-range anisotropic magnetic dipolar interaction. Bosonic polar molecules with much larger electric dipolar interaction are also being considered for BEC experiments [5,9]. Thus one can study the properties of a dipolar BEC with variable short-range interaction [4,7] using a Feshbach resonance [10]. The dipolar BEC [11] with anisotropic long-range atomic interaction has many distinct features [4,5,12–14]. The stability of a dipolar BEC depends on the scattering length as well as the trap geometry [4,12,14]. A disk-shaped trap, with the polarization $\mathbf{z}$ direction perpendicular to the plane of the disk, leads to a repulsive dipolar interaction making the dipolar BEC more stable [4]. On the other hand, a cigar-shaped dipolar BEC oriented along the polarization direction leads to an attractive dipolar interaction and hence may favor a collapse instability [4,14–16]. Also, the anisotropic dipolar interaction leads, in general, to a distinct anisotropic density distribution in a dipolar BEC. The shock and sound waves also propagate with different velocities in different directions in a dipolar BEC [17]. Anisotropic collapse has been observed and studied in a dipolar BEC of $^{52}$Cr atoms [18].

The properties of a BEC have been studied on different types of traps, such as the harmonic trap [1], optical-lattice (OL) trap [19], dichromatic OL trap [20], optical speckle potential trap [21], double-well trap [22], toroidal trap [23,24], and a ring-shaped trap in one [25] and three [26] dimensions, among others. To study the properties of the dipolar BEC, apart from the harmonic trap, the following traps have been used: OL trap [27], dichromatic OL trap [28], toroidal trap [29], and double-well trap [30].

Very recently, there has been an experimental realization of ring-shaped and spherical-shell-shaped traps [31,32]. The ring geometry was created by the time-averaged adiabatic potential resulting from the application of an oscillating magnetic bias field to a radio-frequency-dressed quadrupole trap [32]. The shell geometry was made from a cylindrically symmetric quadrupole field with its symmetry axis aligned with gravity [32]. These geometries of the trap present an opportunity to study the superfluid properties of a BEC in a multiply connected geometry [32] not found in usual traps. In this paper, we study the properties of a dipolar BEC in ring- and shell-shaped traps. The shell-shaped trap is spherically symmetric, whereas the ring-shaped trap is at most axially symmetric. Different orientations of the ring-shaped dipolar BEC with respect to the polarization direction are considered. The stability of the dipolar BEC in these traps is illustrated by phase plots of dipolar and contact interactions. The anisotropic nature of stability properties in a ring-shaped trap is further demonstrated by a consideration of the chemical potential of the system. The ring-shaped dipolar BEC is more stable when the plane of the ring is aligned perpendicular to the polarization direction, than when it is aligned parallel to the polarization direction. In the former case the dipolar interaction is mostly repulsive and in the latter case it is mostly attractive. The anisotropic density distribution of the dipolar BEC in these traps is explicitly demonstrated.

We also consider a vortex dipolar BEC (rotating around the polarization $\mathbf{z}$ direction) of unit angular momentum [33,34] in ring- and shell-shaped traps, when the trapping potential is axially symmetric around the $\mathbf{z}$ direction. In the case of a ring-shaped trap, the axial symmetry is maintained when the ring is in a plane perpendicular to the $\mathbf{z}$ direction. The ring-shaped vortex dipolar BEC is found to be nearly identical to the normal (nonrotating) dipolar BEC for the same sets of parameters. The shell-shaped vortex dipolar BEC is found to possess a distinct density distribution when compared with a normal dipolar BEC.

In Sec. II we describe the ring- and shell-shaped traps and present the mean-field Gross-Pitaevskii (GP) equation which we use to study the normal and vortex dipolar BEC in these traps. In Sec. III we present the numerical results.
obtained by solving the GP equation using the Crank-Nicolson approach. We present stability phase plots of the dipolar BECs in terms of contact and dipolar interactions. The anisotropic density distribution of the BECs, which is a consequence of the anisotropic dipolar interaction, is illustrated for both the traps. The difference in the density distribution between the normal and vortex BECs is also demonstrated. Finally, in Sec. IV we present a brief summary and concluding remarks.

II. ANALYTICAL CONSIDERATION

A trap in the shape of a spherical shell will be taken in the form

\[ V(r) = V_0 \frac{1}{2} m \omega^2 (r - r_0)^2, \]

with \( r = (x, y, z), r = \sqrt{(x^2 + y^2 + z^2)} \), where \( m \) is the mass of an atom, \( r_0 \) is the radius of the shell, \( V_0 \) is the strength of the trap, and \( \omega \) the frequency. For \( r_0 = 0 \), trap (4) reduces to the usual harmonic trap. Similarly, the ring-shaped trap can be written as

\[ V(r) = V_0 \frac{1}{2} m \omega^2 [(\sqrt{x^2 + p^2} - r_0)^2 + q^2], \]

where \( p = (y \cos \alpha + z \sin \alpha), q = (z \cos \alpha - y \sin \alpha), V_0 \) is the strength of the trap, \( \alpha \) is the angle between the polarization direction \( z \) and the perpendicular to the plane of the ring, and \( r_0 \) is the radius of the ring. For \( r_0 = 0 \) and \( \alpha = 0 \) or \( \pi / 2 \), trap (5) reduces to the harmonic trap.

A dilute dipolar BEC of \( N \) atoms, in shell- or ring-shaped traps (4) or (5), will be studied using the following Gross-Pitaevskii (GP) equation [4,12]:

\[ i \frac{\partial \phi(r,t)}{\partial t} = \left[ -\frac{\nabla^2}{2} + V + g|\phi|^2 + g_{dd} F \right] \phi(r,t), \]

with \( g = 4\pi a N, g_{dd} = 3a_{dd} N \). Here the dipolar nonlinearity \( F = \int U_{dd}(r - r')|\phi(r', t)|^2 d^3r', U_{dd}(R) = (1 - 3 \cos^2 \theta)/R^2 \), \( R = r - r' \), normalization \( \int \phi(r)^2 d^3r = 1 \), and \( \theta \) is the angle between \( R \) and the polarization direction \( z \). For the shell trap

\[ V \equiv V_{shell} = V_0 (r - r_0)^2 \]

and for the ring trap

\[ V \equiv V_{ring} = V_0 [(\sqrt{x^2 + p^2} - r_0)^2 + q^2], \]

\[ a_{dd} = \mu_0 \mu_0^2 m/(12 \pi h^2) \] is the strength of dipolar interaction, \( \mu_0 \) is the permeability of free space, and \( \mu \) is the (magnetic) dipole moment. In Eq. (3), length is measured in units of \( l_0 = \sqrt{\hbar/m\omega} \), potential and energies in units of \( \hbar \omega \), and time \( t \) in units of \( l_0 = \omega^{-1} \). In this work we conveniently take \( l_0 = 1 \mu m \), which is the typical unit of length in BEC experiments.

The ring-shaped trap with \( \alpha = 0 \) and the shell-shaped trap are axially symmetric around the \( z \) axis, and a vortex BEC rotating around the \( z \) axis with a conserved angular momentum can be conveniently introduced in these cases. To obtain a quantized vortex of unit angular momentum \( \hbar \) around the \( z \) axis, we introduce a phase (equal to the azimuthal angle) in the wave function [33]. This procedure introduces a centrifugal term \( 1/[2(x^2 + y^2)] \) in the potential of the GP equation so that

\[ V = V + \frac{1}{2(\chi^2 + \chi^2)}, \]

where \( V \) is \( V_{shell} \) for the shell-shaped trap and \( V_{ring} \) for ring-shaped trap with \( \alpha = 0 \). For the ring-shaped trap with \( \alpha \neq 0 \), the potential is not axially symmetric and a conserved angular momentum cannot be defined. We adopt this procedure to study an axially symmetric vortex in a ring- and shell-shaped dipolar BEC.

The chemical potential \( \mu \) of a stationary state propagating as \( \phi(t) \sim \exp(-i\mu t) \) is defined by

\[ \mu = \int \left[ -\frac{1}{2} |\nabla \phi|^2 + V|\phi|^2 + g|\phi|^4 + g_{dd} F|\phi|^2 \right] d^3r. \]

III. NUMERICAL CALCULATION

We numerically solve the 3D GP equation (3) using the split-step Crank-Nicolson method [35]. The dipolar potential is divergent at short distances and hence the treatment of this potential requires some care. The integral over the dipolar potential is evaluated in Fourier (momentum) space by a convolution identity [12] requiring the Fourier transformation of the dipolar potential and density. The Fourier transformation of the dipolar potential can be analytically evaluated [12]. The remaining Fourier transformations are evaluated numerically using a fast Fourier transformation algorithm. In the Crank-Nicolson discretization we used space step 0.1, time step 0.002, and up to 256 space discretization points in each of the three Cartesian directions. We performed an analysis of errors of sizes and energies calculated using our routine and find that the maximum numerical error in the calculation is less than 0.5%.

A. Normal dipolar BEC

In Eqs. (4) and (5), for shell and ring shapes, we take the strength of the potentials \( V_0 = 10 \) and radius \( r_0 = 10 \). This makes reasonably strong traps, so that the width of the shell or ring is small compared to the radius of the shell or ring and the shell and ring shapes of the BECs are pronounced. First we study the stability of the shell- and ring-shaped dipolar BEC. The stability properties of these BECs are best illustrated in phase plots involving the strengths of contact and dipolar nonlinearities \( g \) and \( g_{dd} \), as shown in Fig. 1. For the ring shape, we show two orientations of the ring for \( \alpha = \pi/2 \) and 0, the former corresponding to a ring in a plane parallel to the polarization direction \( z \) and the latter in a plane perpendicular to the polarization direction \( z \). The orientation of the dipoles in the former is quite similar to that in a cigar-shaped BEC along the \( z \) axis in a harmonic trap, and that of the latter is similar to a disk-shaped BEC in an \( x-y \) plane in a harmonic trap. The dipolar interaction contributes predominantly attractively in a cigar configuration with dipoles arranged parallel to the length of the cigar, and it contributes predominantly repulsively in a disk configuration with dipoles arranged perpendicular to the plane of the disk. Hence for a ring-shaped dipolar BEC with \( \alpha = 0 \), the dipolar interaction contributes repulsively and to a positive quantity in energy and chemical potential. On the other hand, for a ring-shaped dipolar BEC with \( \alpha = \pi/2 \), the dipolar interaction contributes attractively and to a negative
quantity in energy and chemical potential. Consequently, for \( \alpha = 0 \), the ring-shaped dipolar BEC is stable for a reasonably large dipolar interaction below a critical value (\( g_{dd} < g_{dd}^{\text{crit}} \)) without any contact interaction (\( g = 0 \)). However, the dipolar BEC without any contact interaction (\( g = 0 \)) collapses for larger dipolar interactions (\( g_{dd} > g_{dd}^{\text{crit}} \)). For \( \alpha = \pi/2 \), the dipolar interaction is mostly attractive, and for a nonzero dipolar interaction, the ring-shaped dipolar BEC is stable only for contact interaction above a critical value, as shown by the phase plot in Fig. 1.

Next we consider the shell-shaped dipolar BEC. In this case the trapping potential is spherically symmetric and unless the dipolar interaction is large compared to the contact interaction, the contribution of the dipolar interaction to the stability of the BEC, and to the chemical potential of the system, is insignificant. However, for a finite \( g_{dd} \) the system collapses unless \( g \) is larger than a critical value. To avoid the collapse, a finite amount of contact repulsion is to be introduced through a finite \( g \), as shown in Fig. 1.

Further consequence of stability characteristics is shown in Fig. 2, where we plot the chemical potential of the dipolar BEC versus \( g \) for different values of \( g_{dd} \). For a ring-shaped dipolar BEC with \( \alpha = \pi/2 \), the dipolar interaction is attractive and contributes negatively to the chemical potential, whereas for \( \alpha = 0 \), the dipolar interaction is repulsive and contributes positively to the chemical potential. Consequently, the chemical potential for \( \alpha = 0 \) is the largest and for \( \alpha = \pi/2 \) is the smallest for a fixed \( g \) and \( g_{dd} \). The chemical potential for \( \alpha = \pi/4 \) lies close to the nondipolar BEC with \( g_{dd} = 0 \), as the contribution of the dipolar term is small in this case. For a shell-shaped dipolar BEC, as noted before, the contribution of the dipolar interaction to the chemical potential is insignificant and the chemical potentials for \( g_{dd} = 0 \) and 200 are practically the same. The dipolar interaction energy nearly vanishes when integrated over all angles in a spherically symmetric density configuration [15] as in the spherical shell. However, in all cases of dipolar BEC (\( g_{dd} = 200 \)), the system collapses for \( g \) less than a critical value \( g_c \) (indicated by an arrow in Fig. 2), where the chemical potential suddenly jumps to an infinitely large negative value corresponding to a collapsed state.

Next we illustrate the structure of a ring-shaped dipolar BEC by three-dimensional (3D) contour plots of density \( |\phi|^2 \). We exhibit the contour density plots of a \(^{164}\text{Dy}\) BEC of 5000 \(^{164}\text{Dy}\) atoms with \( a_{dd} = 130a_0 \). The s-wave scattering length for contact interaction in this case is taken as \( a = 120a_0 \), in close agreement with some experimental estimate [7]. The 3D contour plots of density for \( \alpha = 0, \pi/6, \pi/3, \) and \( \pi/2 \) in this case are shown in Figs. 3(a)–3(d), respectively. For these parameters, in all the plots of Figs. 3, \( g = 399 \) and \( g_{dd} = 103 \). In the plane of the ring, the density is circularly symmetric for \( \alpha = 0 \). However, as the angle \( \alpha \) increases due to the anisotropic dipolar interaction, the density distribution in the plane of the ring is no longer isotropic, as can be seen in Figs. 3(b) and (d).
and 3(c). The anisotropy in density distribution in the ring is visible for \( \alpha = \pi/3 \) in Fig. 3(c) and is most explicit for \( \alpha = \pi/2 \) in Fig. 3(d). Although the dipolar interaction is long range in nature, it is practically zero across the diameter of the ring or the shell (20 \( \mu \text{m} \) or 200 000 \( \AA \)).

In the case of the ring, the density is most asymmetric for \( \alpha = \pi/2 \) and we study the density in this case in some detail for a dipolar BEC of 5000 \( ^{52}\text{Cr} \) atoms with \( g_{dd} = 15a_0 \), and (a) \( a = 20a_0 \), (b) \( a = 50a_0 \), (c) \( a = 70a_0 \), (d) \( a = 100a_0 \).

In Figs. 5(a)–5(d) we show the 3D contour plot of density \( |\phi|^2 \) for \( g_{dd} = 100 \) and different \( g = 300, 600, 1000, \) and 2000. For a clean visualization of the spherical-shell shape, only one half of the full density distribution is shown. The density is most asymmetric in the polarization \( z \) direction in Fig. 5(a) with the smallest contact nonlinearity \( g \), while the dipolar interaction is most prominent. This asymmetry in density reduces as the contact nonlinearity increases, making the anisotropic dipolar interaction less and less pronounced and an almost symmetric density distribution in the plane of the ring is obtained for \( a = 100a_0 \), as can be seen in Fig. 4(d).

The above anisotropic density distribution of the shell-shaped dipolar BEC is further demonstrated by plotting the density along the \( x \), \( z \), and the radial \( r \) directions in Figs. 6(a)–6(d) for \( g_{dd} = 100 \) and \( g = 300, 600, 1000, \) and 2000, respectively. The anisotropy in the density in the three directions is explicitly shown in these figures. The anisotropy clearly reduces as the contact nonlinearity \( g \) increases, making
the dipolar interaction less prominent, as can be seen in Fig. 6(d) with the most isotropic density distribution.

B. Vortex dipolar BEC

Now we study the singly-quantized vortices in ring- and shell-shaped dipolar BECs. In such a vortex, the trapping potential should have azimuthal symmetry. In the ring shape, such symmetry exists only for $\alpha = 0$. However, for $\alpha = 0$ the matter is localized far away from the center [viz. Fig. 3(a)]. Consequently, the added centrifugal part in Eq. (6) is practically zero for large $x$ and $y$ ($\approx 10$), and the density of the vortex state is practically identical with the normal state shown in Fig. 3(a). In the $x$-$y$ plane, both have zero density at the center of the ring. Nevertheless, the phase of the ring vortex wave function of small finite radius changes by $2\pi$ as one moves in a closed contour around the center of the vortex. However, for larger values of angular momentum of the ring-shaped BEC, there could be dissipation when the rotational velocity exceeds a critical value [32,36], larger than the velocity for the unit angular momentum considered here. Below this critical velocity the mass flow has no dissipation in analogy to electrical current in superconductors. Such a persistent flow was observed in a nondipolar BEC in an optically plugged magnetic trap [24].

Next we consider a shell-shaped dipolar BEC rotating around the polarization $z$ direction with unit angular momentum. For this purpose, we solve the GP equation with potential (6). For the vortex state the density on the $z$ axis $|\psi(z)|^2$ becomes zero. Otherwise, the added centrifugal term in Eq. (6) is very small for large $x$ and $y$. For most parts of the shell the values of $x$ and $y$ are large and the centrifugal part of the potential has very little effect on the density of the condensate. Consequently, the density distribution of the dipolar vortex BEC will be very similar to that of the normal BECs shown in Fig. 6, with the only difference that for the vortex the density at all points on the $z$ axis will be zero: $|\psi(z)|^2 = 0$. This is illustrated in Fig. 7, where we plot the densities $|\psi(x)|^2$ and $|\psi(r)|^2$ as in Fig. 6. It is seen that the densities in the $x$ and $r$ directions of the normal and vortex BECs are quite the same. As the density distributions of the normal and vortex BECs are similar, the stability phase plot of Fig. 1 and the chemical potential plot of Fig. 2 for the shell-shaped normal and vortex dipolar BEC are practically the same.

The difference in density distribution between the shell-shaped normal and the vortex BEC can be best studied by considering the isotropic 2D density of the condensate $|\Phi(x,y)|^2 = \int dz |\phi(x,y,z)|^2$ obtained by integrating out the $z$ dependence. For a vortex this 2D density is zero for $x = y = 0$. To illustrate the difference in density distribution of a normal and a vortex BEC, we plot in Fig. 8 the density $|\Phi(x,0)|^2$ versus $x$ for the different cases shown in Fig. 6. For these sets of parameters the densities for the normal and the vortex BECs are shown. The two densities are quite similar over most regions, except near the center $x = 0$. For the vortex BEC the density is zero at the center, whereas for the normal BEC it has a small finite value.

IV. CONCLUSION

We studied the properties of a normal (nonrotating) and vortex dipolar BEC in ring- and shell-shaped traps using the mean-field GP equation. The stability of the system with
anisotropic density distribution, which is a consequence of the anisotropic dipolar interaction, is studied in phase plots of dipolar and contact interactions. The system is more stable with reduced anisotropic density distribution when the dipolar interaction is small compared to the contact interaction. In the shell-shaped trap the dipolar BEC is always unstable when the interaction is zero or attractive. In the ring-shaped trap the dipolar BEC can be stable for zero contact interaction when the plane of the ring makes an angle with the polarization direction ($\alpha \neq \pi/2$), as can be seen from the stability plot in Fig. 1.

The vortex dipolar BECs are also considered in the axially symmetric ring- and shell-shaped traps. The ring-shaped trap is axially symmetric when the ring stays in a plane perpendicular to the polarization direction. In the case of the ring-shaped trap the density distribution of the normal and vortex dipolar BECs is practically the same. The difference in the density distribution of the normal and vortex dipolar BECs in the shell-shaped trap is carefully examined. The experimental realization of the shell- and ring-shaped traps [31,32] and the present theoretical study will trigger further studies of dipolar BEC in these novel traps.

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