Ground-state structure and stability of dipolar condensates in anisotropic traps

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We study the Hartree ground state of a dipolar condensate of atoms or molecules in an three-dimensional anisotropic geometry and at \( T = 0 \). We determine the stability of the condensate as a function of the aspect ratios of the trap frequencies and of the dipolar strength. We find numerically a rich phase space structure characterized by various structures of the ground-state density profile.

I. INTRODUCTION

The realization of Bose-Einstein condensation (BEC) in low-density atomic vapors \cite{1, 2} has led to an explosion of experimental and theoretical research on the physics of quantum-degenerate atomic and molecular systems. While much of the work so far has concentrated on systems characterized by \( s \)-wave two-body interactions, the recent demonstration of a condensate of chromium atoms \cite{3} opens up the study of gases that interact via long-range, anisotropic magnetic dipole interactions. In a parallel development, it can be expected that quantum degenerate samples of heteronuclear polar molecules will soon be available through the use of Feshbach resonances \cite{4, 5}, photoassociation \cite{6, 7}, or a combination of the two. When in their vibrational ground state, these molecules interact primarily via the electric dipole potential, and they are expected to provide a fascinating new type dipole-dominated condensates in the near future.

As a result of the anisotropy and long-range nature of the dipole-dipole interaction, a number of novel phenomena have been predicted to occur in low-density quantum-degenerate dipolar atomic and molecular systems, both in conventional traps and in optical lattices. An early study of the ground state of polar condensates was presented in Ref. \cite{8}, which determined its stability diagram as a function of the number of atoms and \( s \)-wave scattering length. It identified a stable structured ground state for a specific range of parameters. At about the same time, the effect of trap geometry on the stability of the condensate was considered in Ref. \cite{9} for a system dominated by the dipole interaction. This was followed by the prediction \cite{10} of the existence of a number of quantum phases for dipolar bosons in optical lattices. Recent work \cite{11, 12} considers the structural phases of vortex lattices in rotating dipole Bose gases.

A novel feature of dipolar condensates, as compared to their scalar cousins, is the appearance of a roton minimum in their Bogoliubov spectrum. This feature was discussed in the context of atomic condensates in Ref. \cite{13}, which considered the impact of the roton-maxon feature in the excitation spectrum and the stability of pancake-shaped dipolar condensates. For this particular geometry it was found that the excitation spectrum can touch the zero-energy axis for a non-zero wave vector \( \mathbf{k} \), which points to the instability of homogeneous condensates and the onset of density modulations \cite{14}. A roton minimum was also found \cite{15} for the case of laser-induced dipolar interactions in self-bound BECs with cylindrical symmetry. Quasi-2D dipolar bosons with a density-modulated order parameter were determined to be unstable within the mean-field theory \cite{16}, and cigar-shaped quasi-one-dimensional condensates were likewise found \cite{17} to be dynamically unstable for dipoles polarized along the axis of the cylindrical trap. The stability of dipolar condensates in pancake traps was also recently discussed in Ref. \cite{18}, which found the appearance of hiconcave condensates for certain values of the trap aspect ratio and strength of the dipole interaction. From the Bogoliubov excitation spectrum it was possible to attribute the instability of the condensate under a broad range of conditions to its azimuthal component.

Further building on these studies, the present note reports the results of a detailed numerical analysis of the stability and structure of the Hartree ground state of dipolar condensates confined in anisotropic harmonic trap. We proceed by introducing the trap frequencies \( \omega_x, \omega_y \) and \( \omega_z \), respectively, in the \( x, y \) and \( z \) directions, and the corresponding trap aspect ratios \( \lambda_y = \omega_y/\omega_x \) and \( \lambda_z = \omega_z/\omega_x \). Thus \( \lambda_z = 1 \) corresponds to a pancake trap, whereas \( \lambda_z = 0 \) corresponds to a cylindrical trap with free motion in \( z \) direction. We further assume for concreteness that an external field polarizes the dipoles along the \( y \) axis. The stability of the condensate is then determined as a function of the trap aspect ratios and of an effective dipolar interaction strength that is proportional to the number of atoms or molecules in the condensate. Various ground state structures of the condensate are identified in the stable region of parameter space.

The remainder of this paper is organized as follows: Section II introduces our model and comments on important aspects of our numerical approach. Section III summarizes our results, identifying up to five different types of possible ground states, depending on the tightness of the trap and the particle number. Finally, Section IV is a summary and conclusion.

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II. FORMAL DEVELOPMENT

The dipole-dipole interaction between two particles separated by a distance $r$ is

$$V_{dd}(r) = g_{dd} \frac{1 - 3y^2/r^2}{r^3},$$

(1)

where $g_{dd}$ is the dipole-dipole interaction strength and $\hat{y}$ is the polarization direction. For atoms with a permanent magnetic dipole moment we have $g_{dd} = \mu_0 \mu_m^2/4\pi$ while for dipolar molecules $g_{dd} = \mu_0^2/4\pi \epsilon_0 \mu_m$ and $\mu$ being the magnetic moment of the atoms and the electric dipole moment of the molecules, respectively.

Within the mean-field approximation, the condensate order parameter $\phi(r)$ satisfies the Gross-Pitaevskii (GP) equation

$$E\phi(r) = [H_0 + g |\phi^2(r)|] + N \int V_{dd}(r - r') |\phi(r')|^2 d^3r' \phi(r),$$

(2)

where

$$H_0 = -\frac{\hbar^2}{2m} \nabla^2 + \frac{1}{2} m \omega^2 \left(x^2 + \lambda_y^2 y^2 + \lambda_z^2 z^2\right)$$

(3)

is the sum of the kinetic energy and the trapping potential and $N$ denotes the number of particles in the condensate. The second term on the right-hand side of Eq. (2) is the contact interaction, $g = 4\pi \hbar^2 a/m$ being proportional to the s-wave scattering strength $a$, and the third term describes the effects of the nonlocal dipole-dipole interaction. For dipole interaction dominated systems, $g$ is small compared to $V_{dd}$. This is the case that we consider here, and in the following we neglect the s-wave scattering term altogether.

For convenience we introduce the dimensionless parameter

$$D = N g_{dd} m/(\ell_x \hbar^2)$$

(4)

that measures the effective strength of the dipole-dipole interaction, where the oscillator length $\ell_x = \sqrt{\hbar/(m \omega_x)}$. The condensate ground state is then determined numerically by solving the Gross-Pitaevskii equation (2) for imaginary times. The term involving the dipole interaction energy is calculated using the convolution theorem,

$$\int V_{dd}(r - r') |\phi(r')|^2 d^3r' = \mathcal{F}^{-1} \left\{ \mathcal{F} [V_{dd}(r)] \ast \mathcal{F} [|\phi(r)|^2] \right\},$$

where $\mathcal{F}$ and $\mathcal{F}^{-1}$ stand for Fourier transform and inverse Fourier transform, respectively. The dipole-dipole interaction is calculated analytically in momentum space as

$$\mathcal{F} [V_{dd}(r)] = \frac{4\pi}{3} \left[ 3 \frac{k_x^2}{k_x^2 + k_y^2 + k_z^2} - 1 \right],$$

(5)

$k_x, k_y, k_z$ are the momentum components in $x, y, z$ direction.

The initial order parameter was chosen randomly, and the stability diagram was generated for each pair of parameters $(\lambda_y, \lambda_z)$ by increasing the effective dipolar strength $D$ until a critical value $D_{cr}$ above which the condensate collapses. Because of the random initial condition this value varies slightly from run to run. The plotted results show the average over 100 realizations of the initial wave function, the error bars indicating the maximum deviation from of $D_{cr}$ from its mean $D_{cr}$. This approach typically resulted in numerical uncertainties similar to those of Ref. [12].

III. RESULTS

A good starting point for the discussion of our results is the observation that in the case of a cylindrical trap, $\lambda_z = 0$, we found no stable structured condensate ground state. (By structured profiles, we mean profiles that are not simple gaussians.) In particular, solutions exhibiting density modulations along the $z$-axis were found to be unstable. Moving then to the case of a pancake trap by keeping $\lambda_y$ fixed but increasing $\lambda_z$ from 0 to 1, we found for $\lambda_y \gtrsim 4$ the appearance of a small parameter region where the stable ground state is characterized by a structured density profile, the domain of stability of this structured solution increasing with $\lambda_y$. A $\{ \lambda_z - D \}$ phase space stability diagram typical of this regime is shown in Fig. 4 for $\lambda_y = 5$. In this figure, region I is characterized by the existence of a usual condensate with its familiar, structureless gaussian-like density profile. As $\lambda_z$ is increased, the condensate becomes unstable for decreasing values of the effective dipole interaction strength $D$, or alternatively of the particle number $N$. For $5.25 < \lambda_z < 7$, though, the ground state changes from a gaussian-shaped to a double-peaked density profile (domain II in the figure), before the system becomes unstable.

Figures 4 and 5 show surface plots and corresponding 3-D renditions of density profiles typical of the various situations encountered in our study. Figures 4a and 5a are illustrative of the present case. The appearance of two density peaks away from the center of the trap results from the interplay between the repulsive nature of the dipoles in a plane transverse to its polarization direction, the $(x - z)$ plane, and the confining potential.

Increasing the tightness of the trap along the polarization direction $y$, i.e., increasing $\lambda_y$, results in the emergence of additional types of structured ground states. One such case is illustrated in Fig. 5 which is for $\lambda_z = 5.5$. For small values of $\lambda_z$, i.e., a weak trapping potential along the $z$-direction, we observe the appearance of a domain (region III in the figure) characterized by a double-peaked ground state with the maximum density along the $z$ direction and a gaussian-like density in $x$ direction. This type of double-peaked structure along the weak trapping axis was first predicted in Ref. [20].
Typical density profiles in this region resemble those in Figs. 4a and 5a, but with a rotation by 90 degrees in the \((x, z)\)-plane. The regions II and III are separated by a small additional domain IV characterized by a ground-state distribution with a quadruple-peaked structure as illustrated in Figs. 4b and 5b, as might be expected. In general, these characteristics of the ground state density profile persist until \(\lambda_z \approx 6.5\).

Figure 1 shows a stability diagram typical of higher values of the aspect ratio \(\lambda_y\), in this case \(\lambda_y = 7\), for \(0.4 < \lambda_z < 1\). As \(D\) is increased, the ground-state density of the condensate first undergoes a transition from a gaussian-like to a double-peaked profile of the type illustrated in Figs. 4b and 5b (region III). As \(D\) is further increased, this domain is followed for \(\lambda_z\) close enough to unity by a second transition to a domain (region V) with the appearance of a density minimum near trap center. Initially, this minimum is surrounded by a region with a radial density modulation, see Fig. 4c, but for larger values of \(\lambda_z\) this modulation is reduced, see Figs. 4d and 5d. In that region, the density profile resembles the solution previously reported in Ref. 21 for a similar parameter range.

In the case of atoms a typical magnetic moment of \(6\mu_B\), and we find that the range of critical dipole strengths \(D\) corresponding to structured ground states can be achieved for \(10^4 - 10^5\) atoms for trapping frequencies \(\omega_x \approx 1kHz\). For molecules with a typical electric dipole moment of \(1Debye\) the corresponding number is \(10^3 - 10^4\) molecules. While these are relatively high particle numbers, especially for the atomic case, they do not seem out of reach of experimental realization.

\[\text{FIG. 1: } (\lambda_z, D) \text{ stability diagram of a dipolar condensate in an anisotropic trap for } \lambda_y = 5. \text{ The condensate is unstable in the region above the solid line. The dashed line is the boundary between a “structureless gaussian” and a double-peaked ground-state density profile. The error bars give an indication of the accuracy of the numerical simulations.}\]

IV. CONCLUSION

In conclusion, we have performed a detailed numerical study of the ground state structure and stability of ultracold dipolar bosons in an anisotropic trap for dipoles polarized along the \(y\)-direction. The trap aspect ratios along \(y\) and \(z\) direction, \(\lambda_y\) and \(\lambda_z\) were used as control parameters, and the mean-field stability diagram has established as function of these parameters and a dimensionless interaction strength \(D\). For small \(\lambda_y\) the system was found to exhibit a standard density profile, but for larger values, and depending on \(\lambda_z\), various structured ground state were found to appear before reaching the unstable regime where the condensate collapses. These include a four-peak structured solution in the \(x - z\) plane, a ring-like ground state with a modulated radial density profile. For \(\lambda_y \sim 7\) and \(\lambda_z = 1\), we found a biconcave condensate profile, as already reported in [21].

For strong confining potentials along the dipole polarization direction, i.e for large \(\lambda_y\), increasing \(\lambda_z\) can be viewed as resulting in a change from a quasi-one dimensional to a quasi-two-dimensional geometry. As such we can think of the various ground-state structures as a result of dimensional crossover in a trapping geometry. To gain a deeper understanding of these structures as we approach the instability region, future work study the Bogoliubov spectrum of the trapped system.
FIG. 3: Stability diagram of a dipolar condensate in an anisotropic trap with $\lambda_y = 7$, as a function of the dipolar strength $D$ and the aspect ratio $\lambda_z$. The region above the solid line is characterized by unstable ground-state solutions of the mean-field equation. The dashed line marks the boundary between a structured and a gaussian-like ground-state density profile. The dotted line is the boundary between the region with ring-like and two-peaked condensate in $(x-z)$ plane.

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FIG. 4: Two-dimensional surface plots of the structured ground-state density profiles typical of various stable domains: (a) Double-peaked density profile in the \((x - z)\)-plane for region II, for the parameters \(\lambda_y = 5\), \(\lambda_z = .6\) and \(D = 23\). The points of maximum density are away from the trap center and along the \(x\)-direction. In region (III) the shape of the condensate is similar, but with maximum density along \(z\) direction. (b) Typical quadruple-peaked density profile characteristic of region IV. Here \(\lambda_y = 5.5\), \(\lambda_z = .575\) and \(D = 42\). (c) Stable ground state solution in region V with \(\lambda_z < 1\). The density is higher and modulated on a radius away from the trap center in the \(x - z\) plane. In this example \(\lambda_y = 7\), \(\lambda_z = .85\) and \(D = 40\). (d) Density profile typical of the domain V. The condensate is biconcave with maximum density along a constant radius from the trap center. In this example, \(\lambda_y = 7\) and \(D = 32\).

FIG. 5: Three-dimensional ground-state density profile for the same parameters as in Fig. 4.