Radial and Angular Rotons in Trapped Dipolar Gases

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We study Bose-Einstein condensates with purely dipolar interactions in oblate traps. We find that the condensate always becomes unstable to collapse when the number of particles is sufficiently large. We analyze the instability, and find that it is the trapped-gas analogue of the "roton-maxon" instability previously reported for a gas that is unconfined in 2D. In addition, we find that under certain circumstances the condensate wave function attains a biconcave shape, with its maximum density away from the center of the gas. These biconcave condensates become unstable due to azimuthal excitation—an angular roton.

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The realization of a Bose-Einstein condensate (BEC) of ^{52}Cr [1] marks a major development in degenerate quantum gases. The interparticle interaction due to large magnetic dipoles leads to an observable change in the shape of the condensate. In these experiments, the dipolar interaction energy was about 15% of the short-range interaction energy given by the scattering length. It may be expected that advances in using Feshbach resonances [2] to tune the scattering length to zero, will lead in the near future to condensates dominated by pure dipolar interactions. A rich array of intriguing phenomena have been predicted to occur in such a gas. Their properties have been shown to depend crucially on the shape of the trap [3–15]. Roton-like features have been predicted [16,17], along with unique lattice phases [18–20], and vortex structures [21,22]. Dipolar degenerate quantum gases are also attractive as physical implementations of quantum computing [23], and for the study of ultracold chemistry [24].

It is widely agreed that the structure and stability of a dipolar gas will depend critically on the interplay between three factors: the anisotropic dipole-dipole interaction between particles; the anisotropic external potential used to confine the particles; and the number of particles. Still, the details of this interplay remain thus far fragmentary. We take the standard scenario, where the dipoles are assumed to be polarized along a field whose direction defines the laboratory z axis. They are confined by a harmonic trap with cylindrical symmetry about this axis, defined by radial and axial angular frequencies ω_ρ and ω_z, and aspect ratio $\lambda = \omega_z/\omega_\rho$. It has been realized that, because the dipoles would prefer to align in a head-to-tail orientation, the gas elongates in the z direction [3,5]. If this is so, then ultimately the attractive interaction between dipoles should become so large as to initiate a macroscopic collapse as the number of dipoles is increased. In fact, in the large-number limit, one enters the Thomas-Fermi regime, in which a gas with pure dipolar interactions is unstable [10].

The circumstances under which this collapse occurs has been the subject of much discussion. It was argued that for oblate traps with $\lambda > 5.4$, the gas is completely stable, since the trap can overcome the tendency of the gas to elongate along z [4]. However, Ref. [5] found unstable condensates even for $\lambda = 7$. Taking it a step further, Ref. [17] found instabilities even in the $\lambda \to \infty$ limit, by treating a gas that is confined in the z direction, but completely free to move in the transverse plane. The instability was refereed to as a "roton" instability, although the microscopic physics is quite different from the roton-maxon physics in superfluid He. Reference [12] examined the quasi-2D limit of this problem. Rotonlike dispersion curves and supersolidlike phases had earlier been identified in quasi-1D gases, where the dipolar interaction is induced by laser light [16,18,25,26].

In any event, the details of the stability of a pure dipolar gas remain an open question. In this Letter, we revisit this issue, applying a new algorithm which reduces the 3D problem to a 2D one, by using the cylindrical symmetry of the problem [15]. We determine that for any finite of λ, the condensate will decay if sufficiently many dipoles are added. The route toward instability will be shown to exhibit physics similar to the roton mechanism, but adapted to a finite trap environment. Along the way, we demonstrate that stable condensates can have an unusual density profile, where the maximum of density is not in the center.

The dynamics of the condensate wave function is described by the time-dependent Gross-Pitaevskii equation:

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$$i\hbar\frac{\partial\psi(\boldsymbol{r},t)}{\partial t}=\Big[-\frac{\hbar^2}{2M}\nabla^2+\frac{M\omega_\rho^2}{2}(\rho^2+\lambda^2z^2)+(N-1)\frac{4\pi\hbar^2a}{M}|\psi(\boldsymbol{r},t)|^2+(N-1)\times\int d\boldsymbol{r}'V_d(\boldsymbol{r}-\boldsymbol{r}')|\psi(\boldsymbol{r}',t)|^2\Big]\psi(\boldsymbol{r},t), \quad (1)$$

where M is the particle mass and the wave function ψ is normalized to unit norm. The coupling constant for the short-range interaction is proportional to the scattering length a, although we set $a=0$ in the following. The dipole-dipole interaction is given by $V_d(\boldsymbol{r})=d^2(1-3\cos^2\theta)/r^3$, with θ being the angle between the vector $\boldsymbol{r}$ and the z axis. We also define a dimensionless dipolar interaction parameter, $D=(N-1)Md^2/(\hbar^2a_{\rm ho})$, where $a_{\rm ho}=\sqrt{\hbar/M\omega_\rho}$ denotes the transverse harmonic oscillator length. It is convenient to think of increasing D as equivalent to increasing the number of dipoles.

A stable condensate exists when there is a stationary solution of Eq. (1) which is stable to small perturbations. Based on this criterion, we have constructed the stability diagram in Fig. 1, as a function of D and the trap aspect ratio $\lambda=\omega_z/\omega_\rho$. In the figure, the shaded and white areas denote parameter ranges for which the condensate is stable or unstable, respectively. In general, the more pancakelike the trap becomes (larger λ), the more dipoles are required to make the condensate unstable. But eventually, the condensate always becomes unstable for a large enough number of particles. This result is at odds with the conclusion of Ref. [4], but in agreement with that of [5,17]. The reason for the different conclusion of Ref. [4] is not clear, but we find that the for highly pancake traps, a larger grid size, and significantly larger computation time are required to achieve convergence. Moreover, our numerical calculations were facilitated by our new algorithm [15], but we checked that we got the same results using the numerical methods of Ref. [4], provided that we used a large enough grid and strict convergence criterion.

Remarkably, there appear regions in parameter space where the condensate obtains its maximum density away from the center of the trap. These are the darker shaded areas in Fig. 1. The local minimum of the density in the center gives the condensate a biconcave shape, resembling that of a red blood cell (a surface of constant density is illustrated at the top left corner of Fig. 1). A density contour plot of such biconcave condensate is shown in Fig. 2(IIa), with the parameters $\lambda=7$ and $D=30.8$. These structures appear in isolated regions of the parameter space, and, in particular, only for certain aspects ratios in the vicinity of $\lambda\approx 7, 11, 15, 19\ldots$. There seems to be a repeated pattern which probably continues to larger values of λ (although this was not calculated). However, the parameter space area of these regions becomes increasingly small with larger λ, and is already negligible for the fourth region (not shown in Fig. 1). In between the biconcave regions, we find "normal" condensates with maximum density in the center, Fig. 2(Ia). Their density profiles in fact have a fairly sharp peak in the center, as compared to a Gaussian shape.

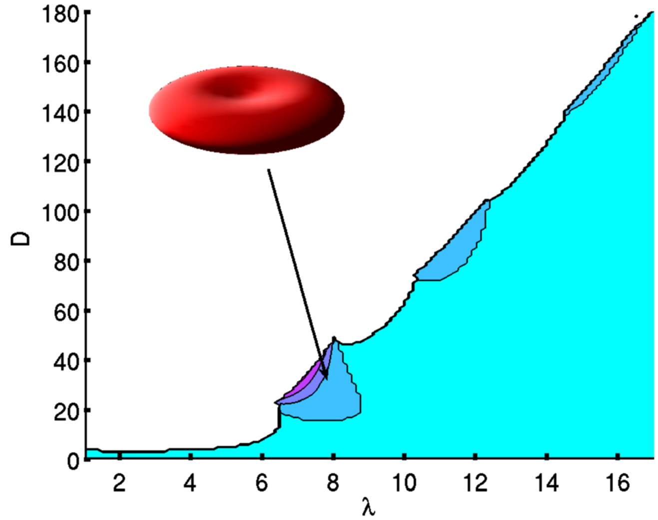

FIG. 1 (color online). Stability diagram of a dipolar condensate in a trap, as a function of the trap aspect ratio $\lambda=\omega_z/\omega_\rho$ and the dipolar interaction parameter D. Shadowed areas are stable, while white unstable against collapse. In the darker, isolated areas, we find biconcave condensates (illustrated with isodensity surface plot at the top right corner) whose maximal density is not at the center. The contours in the biconcave regions indicate the ratio of the central density to the maximal density, with darker areas having a smaller ratio. The contour intervals are 10%, and the minimum ratio obtained is 70%.

To verify the existence of biconcave structures, we solve Eq. (1) numerically both with a 3D algorithm [7] and with our 2D algorithm that exploits the cylindrical symmetry [15], carefully converging both the grid size and resolution. We have also carried out a variational calculation, in which the condensate wave function is taken to be a linear combination of two harmonic oscillator wave functions. The first is a simple Gaussian, and the second is the same Gaussian multiplied by $[H_2(x)+H_2(y)]$, where H_2 is the Hermite polynomial of order 2, and (x, y) are the coordinates perpendicular to the trap axis. Minimizing the variational energy, we find biconcave solutions with a large component of the second wave function, similar in shape to the numerical ones. The exact parameters for appearance of variational biconcave condensates are somewhat different from the numerical ones, and the variational calculation gives a continuous parameter region with biconcave condensates, rather than isolated regions as we find numerically. This is probably due to the oversimplified nature of the variational ansatz.

We find that the existence of islands of biconcave condensates is robust to the addition of small contact interaction, with scattering length a up to $\pm 20\%$ of the dipolar

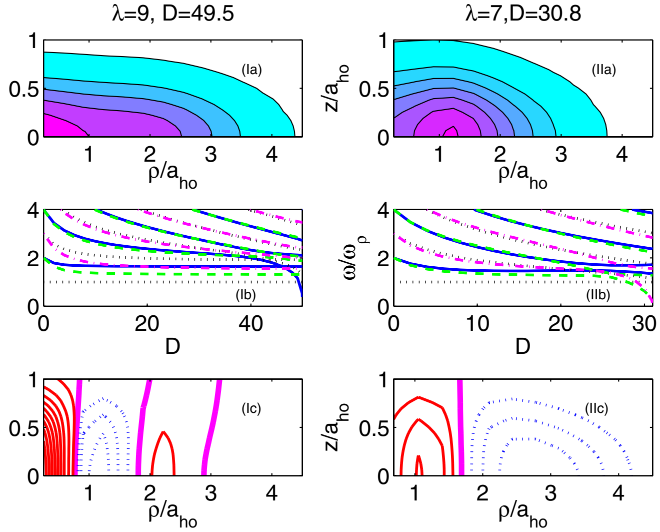

FIG. 2 (color online). (Ia) Contour plot of the ground state density for a dipolar condensate in a trap with aspect ratio $\lambda = 9$ and dipolar interaction strength $D = 49.5$ (close to instability). (IIa) Condensate density contour plot for $\lambda = 7$ and $D = 30.8$. Note the unusual shape, with the maximum of the density occurring away from the center of the trap, along a ring (the plot is a vertical cross section through the cylindrically symmetric condensate). The 3-dimensional shape is biconcave (inset of Fig. 1). (Ib) Excitation spectrum as a function of D for $\lambda = 9$, and (IIb) for $\lambda = 7$. Solid lines are excitation with angular quantum number $m = 0$, dotted lines $m = 1$, dashed lines $m = 2$ and dot-dashed lines $m = 3$. (Ic) The density perturbation (see text) of the lowest excitation mode for the ground state of (Ia), and the corresponding excitation (IIc) for the ground states of (IIa). The heavy lines are nodal lines (actually surfaces in 3D) of the excitation. Red (continuous) contours indicate negative density perturbation and blue (dotted) positive.

length scale given by $Md^2/\hbar^2$. The exact position and size of the islands is sensitive to the size of the scattering length. With negative scattering length, they become larger and move to the right in Fig. 1. The opposite occurs with positive scattering length.

It is perhaps not too surprising that a dipolar condensate could form with the density pushed to the outer rim. After all, the dipoles exert long-range, repulsive forces on one another, and flee to the surface, much as free charges in a conducting material do. What is somewhat more mysterious is why the dipoles do not always behave this way, but rather only for certain well-delineated islands in the stability diagram.

Normally, the condensate properties would be probed experimentally after release from the trap and expansion. However, we have not yet performed simulations of the expansion of the biconcave shaped condensates. One might be able to detect the condensate's shape *in situ*, by using phase-contrast imaging [27].

Condensates with normal and biconcave shapes decay quite differently as the instability boundary is crossed. To examine the collapse mechanism of condensates, we have studied collective excitations in the Bogoliubov–de Gennes (BdG) approximation. Let us first consider the normal case, where the condensate density is a maximum in the center of the trap. An example of this density profile is shown in Fig. 2(Ia). The excitation spectrum for this case is shown in Fig. 2(Ib). The instability of the condensate at $D = 50.0$ coincides with an excited state mode "going soft," i.e., tending to zero excitation frequency. In this case the excited state has zero projection of angular momentum around the z axis, $m = 0$. The excitation consists of a radial nodal pattern, as we show in Fig. 2(Ic) by plotting contours of the eigenmode density $\delta n = u + v$, where u, v are the usual BdG functions [15]. Thus when this condensate becomes unstable, the instability is due to a modulation of the condensate density in the radial direction.

A similar modulation was already considered in the roton instability studied for the infinite-pancake trap [17]. In that case, there is only a trap potential in the z direction, and motion is free in the (x, y) plane, so that the excitations have a definite transverse momentum q in this plane. The instability is expected to occur when this momentum approaches the value $q \approx \hbar/l_z$, where $l_z = \sqrt{\hbar/M\omega_z}$ is the axial confinement length. In this case, excitations in the quasi-2D trap begin to acquire a 3D character and the interparticle repulsion is reduced. For sufficiently many dipoles, the attraction can again overwhelm the condensate and initiate a collapse. Here the instability is a density-wave modulation $\sin(kx)$ with characteristic wavelength $2\pi/k \sim 2\pi l_z$.

For a gas confined in all three dimensions, the same physics appears. For aspect ratio $\lambda = 9$, the axial confinement length is $l_z = a_{\mathrm{ho}}/3$ (recall that the radial oscillator length defines our unit of length). Thus the excited state should posses density-wave oscillations with a wavelength $2\pi l_z \sim 2a_{\mathrm{ho}}$, or nodes at intervals $\sim 1a_{\mathrm{ho}}$. The excitation plotted in Fig. 2(Ic) indeed has radial nodes on approximately this scale. In this sense, the confined gas exhibits what might be termed a "radial roton" instability. In general, the number of the nodal surfaces of the soft mode near the instability increases with λ.

By contrast, for trap aspect ratios such as $\lambda = 7$, where biconcave condensates appear [Fig. 2(IIa)], the lowest excitation mode near the instability boundary has angular momentum projection $m > 0$. For example, $m = 3$ for the case shown [Fig. 2(IIb)], meaning that the excited mode exhibits an azimuthal dependence proportional to $\sin(3\phi)$. Therefore, with increasing number of particles, these condensates collapse due to density modulations in the angular coordinate, which spontaneously break the cylindrical symmetry. Biconcave condensates thus decay to a kind of "angular roton" instability in the trap. [There is also one radial nodal surface, as seen in Fig. 2(IIc). The azimuthal nodal lines are not seen in this (ρ, z) cross section.] The appearance of an angular roton when the ground state has

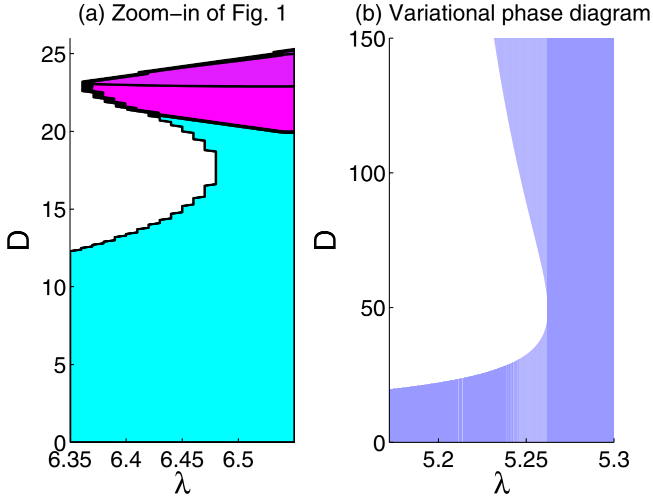

FIG. 3 (color online). (a) Detail of Fig. 1 showing double stability regions. (b) Part of a stability diagram using a Gaussian variational method (there is no area corresponding to biconcave condensates, as they cannot be described by a Gaussian).

biconcave shape may be understood in light of the fact that the maximum density of such a condensate lies a long a ring. The instability may thus also be described as buckling along this ring.

We note that the different excitation spectrum of the biconcave and 'normal' condensates close to the instability boundary may provide an indirect experimental signature for the existence of the biconcave condensates: a low frequency $m > 0$ excitation mode is associated with the later.

Finally, we point out an unusual feature in the stability diagram, shown in Fig. 3: for a small range of aspect ratios $6.36 < \lambda < 6.5$, the boundary between stable and unstable condensates bends back on itself, so that there are two distinct stability regions as D is varied. This feature is also reproduced qualitatively by a variational estimate using a single Gaussian [3(b)]. According to the variational solution, we find that as D increases, the kinetic energy plays a role in destabilizing the condensate. Kinetic energy leads to a tendency to expand more in the tightly confined z direction. In this case, more dipoles can pile up along the axis, where the attraction between them leads to instability. As D increases further, the dipole-dipole interaction becomes more important, and the effects of kinetic energy are mitigated. Finally, in the large-D limit, the Thomas-Fermi regime is reached, and complete instability occurs [10].

In conclusion, we have described the stability diagram for dipolar condensates in pancake traps, found new structured, biconcave condensates, and an excitation spectrum which exhibits a discrete roton-maxon. The soft mode of biconcave condensates near collapse has angular momentum quantum number $m > 0$, giving rise to azimuthal oscillations. This exotic behavior demonstrates the richness of the physics of dipolar condensates.

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