Roton-Maxon Spectrum and Stability of Trapped Dipolar Bose-Einstein Condensates

L. Santos,[1] G.V. Shlyapnikov,[1,2,3] and M. Lewenstein[1]

[1]*Institut für Theoretische Physik, Universität Hannover, D-30167 Hannover, Germany*
[2]*FOM Institute for Atomic and Molecular Physics, Kruislaan 407, 1098 SJ Amsterdam, The Netherlands*
[3]*Russian Research Center Kurchatov Institute, Kurchatov Square, 123182 Moscow, Russia*

(Received 24 January 2003; published 27 June 2003)

We find that pancake dipolar condensates can exhibit a roton-maxon character of the excitation spectrum, so far observed only in superfluid helium. We also obtain a condition for the dynamical stability of these condensates. The spectrum and the border of instability are tunable by varying the particle density and/or the confining potential. This opens wide possibilities for manipulating the superfluid properties of dipolar condensates.

DOI: 10.1103/PhysRevLett.90.250403 PACS numbers: 03.75.Kk, 05.30.Jp

Recent progress in cooling and trapping of polar molecules [1,2] opens fascinating prospects for achieving quantum degeneracy in trapped gases of dipolar particles. Being electrically or magnetically polarized, polar molecules interact with each other via long-range anisotropic dipole-dipole forces. This makes the properties of such dipolar gases drastically different from the properties of commonly studied atomic cold gases, where the interparticle interaction is short range. Other candidates to form a dipolar gas are atoms with large magnetic moments [3,4], and atoms with dc-field- [5] or light-induced electric dipole moments [6–8].

The dipole-dipole interaction is responsible for a variety of novel phenomena in ultracold dipolar systems. The energy independence of the dipole-dipole scattering amplitude for any orbital angular momenta provides realistic possibilities for achieving a superfluid BCS transition in single-component dipolar Fermi gases (see [9] and references therein). Dipolar bosons in optical lattices have been shown to provide a highly controllable environment for engineering various quantum phases [10]. In addition to superfluid and Mott-insulator ones, recently observed in Munich experiments [11] with bosonic atoms, the long-range dipole-dipole potential provides supersolid and checkerboard phases. Dipole-dipole interactions are also responsible for spontaneous polarization and spin waves in spinor condensates in optical lattices [12], and may lead to self-bound structures in the field of a traveling wave [13]. Recently, dipolar particles have been considered as promising candidates for the implementation of fast and robust quantum-computing schemes [8,14].

The long-range and anisotropic (partially attractive) character of dipole-dipole forces ensures a strong dependence of the stability of trapped dipolar Bose-Einstein condensates (BECs) on the trapping geometry [7]. For cylindrical traps with the aspect ratio $l_z/l_\rho > l_* = 0.43$, a purely dipolar condensate is dynamically unstable if the number of particles N exceeds a critical value. A detailed study of the excitation modes for this geometry is contained in Ref. [15]. It has also been argued in Ref. [7] that in pancake traps with $l_z/l_\rho < l_*$ the ground state solution is expected for any N.

In this Letter we analyze the nature of excitations and instability of pancake-shaped dipolar condensates. For this purpose, we consider the physically transparent case of an infinite pancake trap, with the dipoles perpendicular to the trap plane. For the maximum condensate density $n_0 \to \infty$, the dynamical stability requires the presence of a sufficiently large short-range repulsion, in addition to the dipole-dipole interaction. Otherwise, if n_0 exceeds a critical value n_c, excitations with certain (large) in-plane momenta q become unstable. At densities $n < n_c$ the excitation spectrum has a roton-maxon form (see Fig. 1) similar to that in superfluid helium.

The roton-maxon spectrum for helium has been suggested by Landau [16], and later Feynman [17] related the excitation energy to the static structure factor of the liquid. The roton minimum originates from the fact that at intermediate momenta one has a local structure produced by the tendency of atoms to stay apart. The pancake dipolar condensate is the first example of a weakly interacting gas, where the spectrum has a roton-maxon form [18]. We emphasize that the roton-maxon spectrum finds its origin in the momentum dependence of the interparticle interaction. In this sense, it is a general physical phenomenon that should be present in any weakly interacting gas with a similar momentum dependence of the interparticle interaction (scattering amplitude).

In an infinite pancake trap the roton-maxon spectrum allows a transparent physical interpretation. For in-plane momenta q much smaller than the inverse size L of the condensate in the confined direction, excitations have two-dimensional (2D) character. Hence, as the dipoles are perpendicular to the plane of the trap, particles efficiently repel each other and the in-plane excitations are phonons. For $q \gg 1/L$, excitations acquire 3D character and the interparticle repulsion is reduced. This decreases the excitation energy under an increase of q. The energy reaches a minimum and then starts to grow as the excitations continuously enter the single-particle regime.

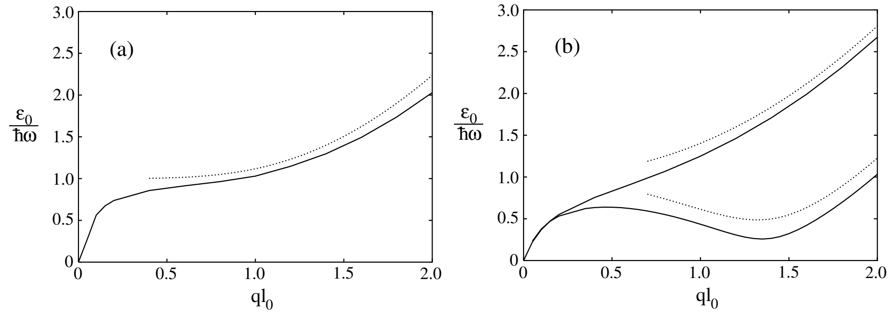

FIG. 1. Dispersion law $\epsilon_0(q)$ for (a) $\beta = 1/2$, $\mu/\hbar\omega = 343$; (b) $\beta = 0.53$, $\mu/\hbar\omega = 46$ (upper curve) and $\beta = 0.47$, $\mu/\hbar\omega = 54$ (lower curve). The solid curves show the numerical results, and the dotted curves the result of Eq. (9).

The minimum energy is zero for the maximum density n_0 equal to a critical value. At higher densities, excitations with momenta q in the vicinity of this minimum become unstable and the condensate collapses. Below we find the condensate wave function, excitation spectrum, and the conditions for both rotonization and instability.

We consider a condensate of dipolar particles harmonically confined in the direction of the dipoles (z) and uniform in two other directions ($\boldsymbol{\rho} = \{x, y\}$). The dynamics of the condensate wave function $\psi(\mathbf{r}, t)$ in this infinite pancake trap is described by the time-dependent Gross-Pitaevskii (GP) equation (see [7] and references therein),

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r}, t) = \left\{-\frac{\hbar^2}{2m}\Delta + \frac{m}{2}\omega^2 z^2 + g|\psi(\mathbf{r}, t)|^2 + d^2\int d\mathbf{r}' V_d(\mathbf{r} - \mathbf{r}')|\psi(\mathbf{r}', t)|^2\right\}\psi(\mathbf{r}, t), \tag{1}$$

where ω is the confinement frequency, m is the particle mass, and d the dipole moment. The wave function $\psi(\mathbf{r}, t)$ is normalized to the total number of particles. The third term in the right-hand side (rhs) of Eq. (1) corresponds to the mean field of short-range (van der Waals) forces, and the last term to the mean field of the dipole-dipole interaction. The coupling constant for the short-range interaction is g, and $V_d(\vec{r}) = (1 - 3\cos^2\theta)/r^3$ is the potential of the dipole-dipole interaction, with θ being the angle between the vector $\vec{r}$ and the direction of the dipoles (z).

The ground state wave function is independent of the in-plane coordinate $\boldsymbol{\rho}$ and can be written as $\psi_0(z)\exp(-i\mu t)$, where μ is the chemical potential. Then, integrating over $d\boldsymbol{\rho}'$ in the dipole-dipole term of Eq. (1), we obtain a one-dimensional equation similar to the GP equation for short-range interactions:

$$\left\{-\frac{\hbar^2}{2m}\Delta + \frac{m}{2}\omega^2 z^2 + (g + g_d)\psi_0^2(z) - \mu\right\}\psi_0(z) = 0, \tag{2}$$

where $g_d = 8\pi d^2/3$. We will discuss the case of $(g + g_d) > 0$, where the chemical potential μ is always positive. For $\mu \gg \hbar\omega$ the condensate presents a Thomas-Fermi (TF) density profile in the confined direction: $\psi_0^2(z) = n_0(1 - z^2/L^2)$, with $n_0 = \mu/(g + g_d)$ being the maximum density, and $L = (2\mu/m\omega^2)^{1/2}$ the TF size.

Linearizing Eq. (1) around the ground state solution $\psi_0(z)$ we obtain the Bogoliubov–de Gennes (BdG) equations for the excitations. Those are characterized by the momentum $\mathbf{q}$ of the in-plane free motion and by an integer quantum number ($j \geq 0$) related to the motion in the z direction. The excitation wave functions take the form $f_\pm(z)\exp(i\mathbf{q}\boldsymbol{\rho})$, where $f_\pm = u \pm v$, and u, v are the Bogoliubov $\{u, v\}$ functions. Then the BdG equations read

$$\epsilon f_- = \frac{\hbar^2}{2m}\left[-\frac{d^2}{dz^2} + q^2 + \frac{\Delta\psi_0}{\psi_0}\right]f_+ \equiv H_{\rm kin}f_+, \tag{3}$$

$$\epsilon f_+ = H_{\rm kin}f_- + H_{\rm int}[f_-], \tag{4}$$

where $H_{\rm kin}$ is the sum of kinetic energy operators, and

$$H_{\rm int}[f_-] = 2(g_d + g)f_-(z)\psi_0^2(z) - (3/2)g_d\, q\, \psi_0(z)\int_{-\infty}^{\infty} dz' f_-(z')\psi_0(z') \times \exp(-q|z - z'|). \tag{5}$$

For each j we get the excitation energy ϵ_j as a function of q. We will be mostly interested in the lowest excitation branch $\epsilon_0(q)$ for which the confined motion is not excited in the limit $q \to 0$.

The second term in the rhs of Eq. (5) originates from the nonlocal character of the dipole-dipole interaction and gives rise to the momentum dependence of an effective coupling strength. In the limit of low in-plane momenta $qL \ll 1$, this term can be omitted. In this case, excitations of the lowest branch are essentially 2D and the effective coupling strength corresponds to repulsion. Equations (3) and (4) become identical to the BdG equations for the excitations of a trapped condensate with a short-range interaction characterized by a coupling constant $(g + g_d) > 0$. In the TF regime for the confined motion, the spectrum of low-energy excitations for this case has been found by Stringari [19]. The lowest branch represents phonons propagating in the x, y plane. The dispersion law and the sound velocity c_s are given by

$$\epsilon_0(q) = \hbar c_s q; \qquad c_s = (2\mu/3m)^{1/2}. \qquad (6)$$

For $qL \gg 1$, the excitations become 3D and the effective coupling strength decreases. The interaction term is then reduced to $H_{\rm int}[f_-] = (2g - g_d)\psi_0^2(z)f_-(z)$; as in the integrand of Eq. (5) one can put $z' = z$ in the arguments of f_- and ψ_0. In this case, Eqs. (3) and (4) are similar to the BdG equations for the excitations of a condensate with short-range interactions characterized by a coupling constant $(2g - g_d)$. If the parameter $\beta = g/g_d > 1/2$, this coupling constant is positive and one has excitation energies which are real and positive for any momentum q and condensate density n_0. For $\beta < 1/2$, the coupling constant is negative and one easily shows that at sufficiently large density the condensate becomes unstable. For collective excitations in the TF regime at $n_0 \to \infty$, kinetic energy terms in Eq. (4) can be omitted, and it reads $\epsilon f_+ = (2g - g_d)n_0(z)f_-$. Then, rescaling the excitation energies as $\epsilon^2 = \tilde{\epsilon}^2(2g - g_d)/(g + g_d)$, Eqs. (3) and (4) give the eigenmode equation $\tilde{\epsilon}^2 f_+ = 2(g + g_d)n_0(z)H_{\rm kin}f_+$ for positive excitation energies $\tilde{\epsilon}$ in the case of short-range repulsive interaction with the coupling constant $(g + g_d)$. Thus, for $\beta < 1/2$ we obtain $\epsilon^2 < 0$ and imaginary ϵ, which indicates dynamical instability of the condensate with regard to these high-momentum excitations.

We thus see that the most interesting behavior of the excitation spectrum in the TF regime is expected for $qL \gg 1$ and β close to the critical value 1/2. In our analytical analysis we first reduce Eqs. (3) and (4) to the equation for the function W defined by the relation $f_+ = W\sqrt{1 - x^2}$, where $x = z/L$. Expressing the function f_- through W from Eq. (3), we substitute it into Eq. (4) and integrate straightforwardly over dz' in $H_{\rm int}[f_-]$ as the main contribution to the integral comes from a narrow range of distances $|z' - z| \sim 1/q$. This yields

$$\left[\frac{1}{2}(1 - x^2)\frac{d^2W}{dx^2} - \left(1 + \frac{3}{2(1+\beta)}\right)x\frac{dW}{dx}\right]\hbar^2\omega^2 + \left[\epsilon^2 - E_q^2 - \frac{2\beta - 1}{1 + \beta}\mu E_q(1 - x^2) - \frac{3\hbar^2\omega^2}{2(1+\beta)}\right]W = 0, \qquad (7)$$

where $E_q = \hbar^2 q^2/2m$. Here we omitted terms of the order of $E_q\hbar^2\omega^2/\mu$ and $\hbar^4\omega^4/\mu^2$, since they are small compared to either $\hbar^2\omega^2$ or E_q^2.

For each mode of the confined motion (each quantum number j), the solution of Eq. (7) can be written as series of expansion in Gegenbauer polynomials $C_n^\lambda(x)$, where $\lambda = (4 + \beta)/2(1 + \beta)$, and $n \geq 0$ is an integer. The coupling between polynomials of different power is provided by the term proportional to $(2\beta - 1)(1 - x^2)W$. For the critical value $\beta = 1/2$ the coupling is absent, and we then obtain $W_j \propto C_j^\lambda(x)$. The dispersion law is characterized by a plateau [see Fig. 1(a)], and for the jth branch of the spectrum it is given by

$$\epsilon_j^2(q) = E_q^2 + \hbar^2\omega^2[1 + j(j + 3)/2]. \qquad (8)$$

For $\beta \neq 1/2$, assuming that the coupling term $\mu E_q|2\beta - 1|/(1 + \beta) \lesssim \hbar^2\omega^2$ and it does not significantly modify the eigenfunctions, we can still confine ourselves to the perturbative approach. Then, as the polynomials C_j^λ are orthogonal with the weight $(1 - x^2)^{\lambda - 1/2}$, for the lowest branch of the spectrum we obtain

$$\epsilon^2(q) = E_q^2 + \frac{(2\beta - 1)(5 + 2\beta)}{3(1 + \beta)(2 + \beta)}E_q\mu + \hbar^2\omega^2. \qquad (9)$$

From Eq. (9) one sees two types of behavior of the spectrum. For $\beta > 1/2$ the excitation energy monotonously increases with q [see Fig. 1(b)]. If $\beta < 1/2$, then the dispersion law (9) is characterized by the presence of a minimum. Since in the limit of $qL \ll 1$ the energy ϵ_0 grows with q, the existence of this minimum indicates that the spectrum as a whole should have a roton-maxon character [see Fig. 1(b)]. This behavior is known from the physics of liquid helium. As discussed above, in our case it is related to the reduction in the coupling strength with an increase of momentum, resulting from the transformation of the character of excitations from 2D to 3D.

As follows from Eq. (9) for β close to 1/2, the roton minimum is located at $q = (16\mu\delta/15\hbar\omega)^{1/2}1/l_0$, where $\delta = 1/2 - \beta$, and $l_0 = (\hbar/m\omega)^{1/2}$ is the harmonic oscillator length for the confined motion. The excitation energy at this point is $\epsilon_{\rm min} = [\hbar^2\omega^2 - (8\mu\delta/15)^2]^{1/2}$. An increase of the density (chemical potential) or δ makes the roton minimum deeper. For $\mu\delta/\hbar\omega = 15/8$ the minimum energy reaches zero at $q = \sqrt{2}/l_0$. At larger values of $\mu\delta/\hbar\omega$ one gets imaginary excitation energies for $q \sim 1/l_0$, and the condensate becomes unstable.

We have then found the excitation spectrum numerically from Eqs. (3) and (4) for various values of β and $\mu/\hbar\omega$. The results for the TF regime and β close to 1/2 are presented in Fig. 1, where one sees a good agreement between the numerics and analytics. The discrepancy is mainly due to the neglect of the border effects and some of the kinetic energy terms when obtaining Eq. (7) from Eqs. (3) and (4). A similar behavior of the spectrum is observed for non-TF condensates. In this case, due to a large kinetic energy in the confined direction, the stability of the condensate does not require as strong a short-range repulsive coupling strength as in the TF regime. Accordingly, the rotonization of the spectrum and the instability appear at smaller values of β. These critical β have been calculated numerically as functions of $\mu/\hbar\omega$ and are shown in Fig. 2.

The dipolar condensate is the first example of a weakly interacting gas offering a possibility of obtaining a roton-maxon dispersion, up to now observed only in the relatively more complicated physics of liquid He. In contrast

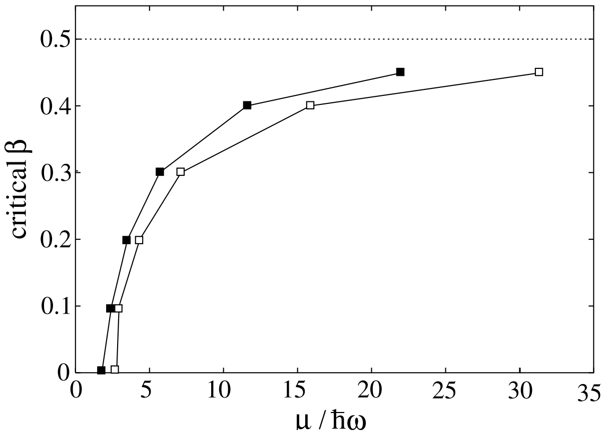

FIG. 2. Critical values of β for the rotonization (filled squares) and for the instability (hollow squares) versus $\mu/\hbar\omega$.

to the helium case, the rotonization in dipolar condensates is *tunable*. By varying the density, the frequency of the tight confinement, and the short-range coupling, one can manipulate and control the spectrum, making the roton minimum deeper or shallower. One can also eliminate it completely and get the Bogoliubov-type spectrum or, on the opposite, reach the point of instability.

The instability of dipolar condensates with regard to short-wave excitations is fundamentally different from the well-known instability of condensates with attractive short-range interaction (negative scattering length). In the latter case the chemical potential is negative and the ground state does not exist. The unstable excitations are long wave, and an infinitely large cloud undergoes local collapses. For the dipolar BEC the chemical potential is positive and the instability is related to the momentum dependence of an effective coupling strength. The unstable excitations become the ones with high momenta at which the coupling is attractive. The existence of the roton minimum at a given $\beta < 1/2$ for $\mu/\hbar\omega$ just below the point of instability is likely to indicate that there is a new ground state in the region of the condensate instability. The presence and character of this state will be a subject of our future studies.

The presence of the roton minimum in the excitation spectrum can be observed in Bragg-spectroscopy experiments [20] or in measurements of the critical superfluid velocity [21]. According to the Landau criterion [22], the critical velocity v_c is equal to the minimum value of $\epsilon_0(q)/q$, and the presence of the roton minimum strongly reduces v_c. Even in the absence of rotonization, a decrease in the slope of the dispersion curve at large momenta leads to a significant reduction of the critical velocity.

In conclusion, we have found that pancake dipolar condensates can exhibit a roton-maxon character of the excitation spectrum. The presence, position, and depth of the roton minimum are tunable by varying the density, confining potential, and the short-range coupling strength. This opens new handles on manipulations of superfluid properties of trapped condensates.

We acknowledge support from Deutsche Forschungsgemeinschaft, the Alexander von Humboldt Foundation, the RTN Cold Quantum Gases, ESF PESC BEC2000+, the Dutch Foundations FOM and NWO, INTAS, and the Russian Foundation for Fundamental Research.

[1] J. D. Weinstein *et al.*, Nature (London) **395**, 148 (1998); J. M. Doyle and B. Friedrich, Nature (London) **401**, 749 (1999).

[2] H. L. Bethlem, G. Berden, and G. Meijer, Phys. Rev. Lett. **83**, 1558 (1999); H. L. Bethlem *et al.*, Phys. Rev. Lett. **84**, 5744 (2000); H. L. Bethlem *et al.*, Nature (London) **406**, 491 (2000); H. L. Bethlem *et al.*, Phys. Rev. A **65**, 053416 (2002).

[3] J. D. Weinstein *et al.*, Phys. Rev. A **57**, R3173 (1998); J. Stuhler *et al.*, *ibid.* **64**, 031405 (2001).

[4] K. Góral, K. Rzążewski, and T. Pfau, Phys. Rev. A **61**, 051601 (2000).

[5] S. Yi and L. You, Phys. Rev. A **61**, 041604 (2000); **63**, 053607 (2001); **66**, 013607 (2002).

[6] D. O'Dell, S. Giovanazzi, G. Kurizki, and V. M. Akulin, Phys. Rev. Lett. **84**, 5687 (2000).

[7] L. Santos, G.V. Shlyapnikov, P. Zoller, and M. Lewenstein, Phys. Rev. Lett. **85**, 1791 (2000).

[8] D. Jaksch *et al.*, Phys. Rev. Lett. **85**, 2208 (2000).

[9] M. A. Baranov, M. S. Mar'enko, V. S. Rychkov, and G.V. Shlyapnikov, Phys. Rev. A **66**, 013606 (2002).

[10] K. Góral, L. Santos, and M. Lewenstein, Phys. Rev. Lett. **88**, 170406 (2002).

[11] M. Greiner *et al.*, Nature (London) **415**, 39 (2002).

[12] H. Pu, W. Zhang, and P. Meystre, Phys. Rev. Lett. **87**, 140405 (2001); W. Zhang, H. Pu, C. Search, and P. Meystre, *ibid.* **88**, 060401 (2002).

[13] S. Giovanazzi, D. O'Dell, and G. Kurizki, Phys. Rev. Lett. **88**, 130402 (2002).

[14] G. K. Brennen, C. M. Caves, P. S. Jessen, and I. H. Deutsch, Phys. Rev. Lett. **82**, 1060 (1999); G. K. Brennen, I. H. Deutsch, and C. J. Williams, Phys. Rev. A **65**, 022313 (2002); D. DeMille, Phys. Rev. Lett. **88**, 067901 (2002).

[15] K. Góral and L. Santos, Phys. Rev. A **66**, 023613 (2002).

[16] L. Landau, J. Phys. U.S.S.R. **11**, 91 (1947).

[17] R. P. Feynman, Phys. Rev. **94**, 262 (1954).

[18] Recently, a roton-maxon dispersion has been independently calculated for some particular cases in elongated cigar-shaped condensates with laser-induced dipole-dipole interatomic interactions: D. O'Dell, S. Giovanazzi, and G. Kurizki, Phys. Rev. Lett. **90**, 110402 (2003).

[19] S. Stringari, Phys. Rev. A **58**, 2385 (1998).

[20] J. Steinhauer, R. Ozeri, N. Katz, and N. Davidson, Phys. Rev. Lett. **88**, 120407 (2002).

[21] A. P. Chikkatur *et al.*, Phys. Rev. Lett. **85**, 483 (2000).

[22] E. M. Lifshitz and L. P. Pitaevskii, *Statistical Physics II* (Pergamon Press, New York, 1989).