

## Bose-Einstein Condensation in Trapped Dipolar Gases

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We discuss Bose-Einstein condensation in a trapped gas of bosonic particles interacting dominantly via dipole-dipole forces. We find that in this case the mean-field interparticle interaction and, hence, the stability diagram are governed by the trapping geometry. Possible physical realizations include ultracold heteronuclear molecules, or atoms with laser induced electric dipole moments.

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Bose-Einstein condensation (BEC) of trapped atomic gases [1,2] offers unique possibilities to highlight a general physical problem of how the nature and stability of a Bose-condensed state is influenced by the character of interparticle interaction. In this respect, especially interesting are ultracold gases with attractive interaction between particles (scattering length  $a < 0$ ). As known [3], spatially homogeneous condensates with  $a < 0$  are absolutely unstable with regard to local collapses. The presence of the trapping field changes the situation drastically. This has been revealed in the successful experiments at Rice [2] on BEC of magnetically trapped atomic  ${}^7\text{Li}$  ( $a = -14 \text{ \AA}$ ). As found in theoretical studies [3], if the number of condensed particles is sufficiently small (of order  $10^3$  in the Rice experiments) and the spacing between the trap levels exceeds the mean-field interparticle interaction  $n_0|g|$  ( $n_0$  is the condensate density,  $g = 4\pi\hbar^2 a/M$ , where  $M$  is the atom mass), there will be a metastable Bose-condensed state. In other words, the condensate is stabilized if the negative pressure caused by the interparticle attraction is compensated by the quantum pressure imposed by the trapping potential. In some sense, this is similar to the gas-liquid phase transition in a classical system with interparticle attraction: The gas phase is stable as long as the thermal pressure exceeds the (negative) interaction-induced pressure (see [4]).

The recent success in creating ultracold molecular clouds [5–7] opens fascinating prospects to achieve quantum degeneracy in trapped gases of heteronuclear molecules. In a sufficiently high electric field “freezing” their rotational motion, these molecules interact via the dipole-dipole forces. This interaction is long range and anisotropic (partially attractive), and there is a nontrivial question of achieving BEC and manipulating condensates in trapped gases of dipolar particles.

Thus far, only the interaction between (small) atomic dipoles has been included in the discussion of the condensate properties. Góral *et al.* [8] considered the effect of magnetic dipole interaction in a trapped spin-polarized atomic condensate. Magnetic dipoles are small (of the order the Bohr magneton  $\mu_B$ ), and even for atoms like chromium ( $6\mu_B$ ) the magnetic interactions are dominated

by the van der Waals forces. Nevertheless, for a relatively small scattering length  $a$  the condensate wave function may develop novel structures reflecting the interplay between the two types of forces. These effects can be amplified by modifying  $a$ , which hopefully will soon become a standard technique [9], and could eventually appear in other systems, such as polar molecules, as pointed out in Ref. [8]. Similar effects have been discussed by Yi and You [10] for ground-state atoms with electric dipole moments induced by a high dc field (of the order of  $10^6 \text{ V/cm}$ ). These authors have demonstrated the validity of the Gross-Pitaevskii equation (GPE) for this system, constructed the corresponding pseudopotential, and determined an effective scattering length.

In this Letter we discuss BEC in a trapped gas of dipolar particles, where the interparticle interaction is dominated by the dipole-dipole forces. Possible realizations include the (electrically polarized) gas of heteronuclear molecules as they have large permanent electric dipoles. We also propose a method of creating a polarized atomic dipolar gas by laser coupling of the atomic ground state to an electrically polarized Rydberg state. We assume that the interparticle interaction is not obscured by short-range forces and by the shape resonances of the dipole-dipole potential (cf. [10]). Then, similar to the condensates with  $a < 0$ , dipolar condensates are unstable in the spatially homogeneous case, and can be stabilized by confinement in a trap. However, we find a striking difference from common atomic condensates: In the BEC regime the sign and the value of the dipole-dipole interaction energy in the system is strongly influenced by the trapping geometry and, hence, the stability diagram depends crucially on the trap anisotropy. This offers new possibilities for controlling and engineering macroscopic quantum states. For dipoles oriented along the axis of a cylindrical trap we have found a critical value  $l_* = 0.4$  for the square root of the ratio of the radial to axial frequency  $l = (\omega_\rho/\omega_z)^{1/2}$ : Pancake traps with  $l < l_*$  mostly provide a repulsive mean field of the dipole-dipole interaction, and thus the dipolar condensate in these traps will be stable at any number of particles  $N$ . For  $l > l_*$  the stability requires  $N < N_c$ , where the critical

value  $N_c$  at which the collapse occurs is determined by the condition that (on average) the mean-field interaction is attractive and close to  $\omega_\rho$ .

We consider a condensate of dipolar particles in a cylindrical harmonic trap. All dipoles are assumed to be oriented along the trap axis. Accordingly, the dipole-dipole interaction potential between two dipoles

is given by  $V_d(\mathbf{R}) = (d^2/R^3)(1 - 3\cos^2\theta)$ , where  $d$  is the dipole moment,  $\mathbf{R}$  the distance between the dipoles, and  $\theta$  the angle between the vector  $\mathbf{R}$  and the dipole axis. The potential  $V_d(\mathbf{R})$  is long range, and one cannot use the pseudopotential approach for the mean field. Similar to [8,10], we describe the dynamics of the condensate wave function  $\psi(\mathbf{r}, t)$  by using the time-dependent GPE

$$i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r}, t) = \left\{ -\frac{\hbar^2}{2m} \nabla^2 + \frac{M}{2} (\omega_\rho^2 \rho^2 + \omega_z^2 z^2) + g|\psi(\mathbf{r}, t)|^2 + d^2 \int d\mathbf{r}' \frac{1 - 3\cos^2\theta}{|\mathbf{r} - \mathbf{r}'|^3} |\psi(\mathbf{r}', t)|^2 \right\} \psi(\mathbf{r}, t). \quad (1)$$

Here  $\psi(\mathbf{r}, t)$  is normalized to the total number of condensate particles  $N$ . The third term in the right-hand side corresponds to the mean field of short-range (van-der-Waals-like) forces, and the last term to the mean field of the dipole-dipole interaction. We omit the term  $g|\psi(\mathbf{r}, t)|^2\psi(\mathbf{r}, t)$ , assuming that the interparticle interaction is dominated by the dipole-dipole forces, and the system is away from the shape resonances of  $V_d(\mathbf{R})$  ( $d^2 \gg |g| = 4\pi\hbar^2|a|/M$ ).

The wave function of the relative motion of a pair of dipoles is influenced by the dipole-dipole interaction at interparticle distances  $|\mathbf{r} - \mathbf{r}'| \lesssim r_* = Md^2/\hbar^2$ . This influence is ignored in the dipole-dipole term of Eq. (1), as the main contribution to the integral comes from distances  $|\mathbf{r} - \mathbf{r}'|$  of order the spatial size of the condensate, which we assume to be much larger than  $r_*$ .

Away from the shape resonances, the dipolar condensate is unstable in the spatially homogeneous case. For all dipoles parallel to each other, by using the Bogolyubov method one easily finds the anisotropic dispersion law for elementary excitations:  $\varepsilon(\mathbf{k}) = [E_k^2 + 8\pi E_k n_0 \times d^2(\cos^2\theta_k - 1/3)]^{1/2}$ , where  $E_k = \hbar^2 k^2/2M$ ,  $n_0$  is the condensate density, and  $\theta_k$  the angle between the excitation momentum  $\mathbf{k}$  and the direction of the dipoles. The instability is clearly seen from the fact that at small  $k$  and  $\cos^2\theta_k < 1/3$  one has imaginary excitation energies  $\varepsilon$ .

To understand the influence of the trapping field on the dipolar condensate, we have simulated Eq. (1) for various values of the number of particles  $N$ , dipole moment  $d$ , and the trap aspect ratio  $l$ . By evolving Eq. (1) in imaginary time, we have found the condition under which the condensate is stabilized by the trapping field and investigated static properties of this Bose-condensed state.

For the stationary condensate the wave function  $\psi(\mathbf{r}, t) = \psi_0(\mathbf{r})\exp(-i\mu t/\hbar)$ , where  $\mu$  is the chemical potential, and the left-hand side of Eq. (1) becomes  $\mu\psi_0(\mathbf{r})$ . The important energy scales of the problem are the trap frequencies  $\omega_z$ ,  $\omega_\rho$ , and the dipole-dipole interaction energy per particle, defined as  $V = (1/N) \int V_d(\mathbf{r} - \mathbf{r}')\psi_0^2(\mathbf{r})\psi_0^2(\mathbf{r}') d\mathbf{r} d\mathbf{r}'$ . Accordingly, the quantity  $V/\hbar\omega_\rho$ , the aspect ratio of the trap  $l$ , and the (renormalized) number of particles  $\sigma = Nr_*/a_{\max}$  [with  $a_{\max} = (\hbar/2M\omega_{\min})^{1/2}$  being the maximal oscillator length of the trap] form the necessary set of parameters allowing us to determine the chemical potential and give a full description of the behavior of a trapped dipolar condensate.

We have found that the dipolar condensate is stable either at  $V > 0$ , or at  $V < 0$  with  $|V| < \hbar\omega_\rho$ . This requires  $N < N_c$ , where the critical number  $N_c$  depends on the trap aspect ratio  $l$ . The calculated dependence  $N_c(l)$  is presented in Fig. 1 and clearly indicates the presence of a critical point  $l_* = 0.4$ . In pancake traps with  $l < l_*$  the condensate is stable at any  $N$ , because  $V$  always remains positive (see Fig. 2). For small  $N$  the shape of the cloud is Gaussian in all directions. With increasing  $N$ , the quantity  $V$  increases and the cloud first becomes Thomas-Fermi in the radial direction and then, for a very large  $N$ , also axially. The ratio of the axial to radial size of the cloud,  $L = L_z/L_\rho$ , continuously decreases with increasing number of particles and reaches a limiting value at  $N \rightarrow \infty$  (see Fig. 3). In this respect, for a very large  $N$  we have a pancake Thomas-Fermi condensate.

For  $l \geq 1$  the mean-field dipole-dipole interaction is always attractive. The quantity  $|V|$  increases with  $N$  and the shape of the cloud changes (see Figs. 2 and 3). In spherical traps the cloud becomes more elongated in the axial direction and near  $N = N_c$  the shape of the cloud is close to Gaussian, with the aspect ratio  $L = 2.1$ . In cigar-shaped traps ( $l \gg 1$ ) especially interesting is the regime where  $\hbar\omega_z \ll |V| \ll \hbar\omega_\rho$ . In this case the radial shape of the cloud remains the same Gaussian as in a noninteracting gas, but the axial behavior of the condensate will be governed by the dipole-dipole interaction which acquires a quasi-1D character. Thus, one has a (quasi)1D gas with attractive interparticle interaction and is dealing with a stable

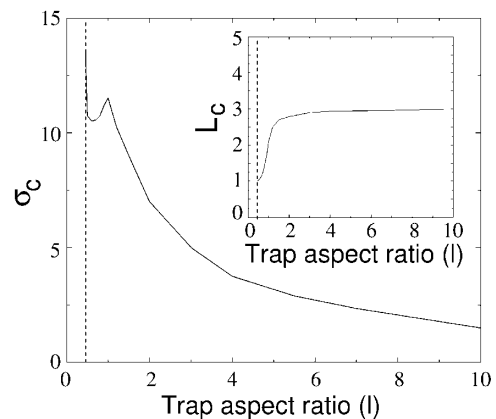


FIG. 1. Critical value  $\sigma_c = N_c r_*/a_{\max}$  and (in the inset) the corresponding condensate aspect ratio  $L_c$  versus  $l$ .

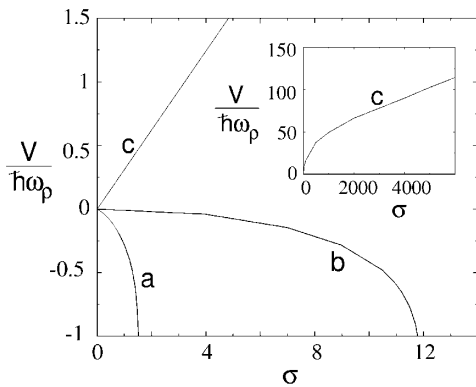


FIG. 2. Dipole-dipole interaction energy  $V$  versus  $\sigma$  for (a)  $l = 10$ , (b)  $l = 1$ , and (c)  $l = 0.1$ .

(bright) solitonlike condensate where attractive forces are compensated by the kinetic energy [11]. With increasing  $N$ ,  $L_z$  decreases. Near  $N = N_c$ , where  $|V|$  is close to  $\hbar\omega_\rho$ , the axial shape of the cloud also becomes Gaussian and the aspect ratio takes the value  $L \approx 3.0$ . For  $l_* \leq l < 1$ , the dipole-dipole interaction energy is positive for a small number of particles and increases with  $N$ . The quantity  $V$  reaches its maximum, and the further increase in  $N$  reduces  $V$  and makes the cloud less pancake. At the critical point  $N = N_c$  the shape of the cloud is close to Gaussian and the aspect ratio  $L < 3.0$ , tending to 1 as  $l \rightarrow l_*$ .

To gain insight into the nature of the stability of dipolar condensates in pancake traps we performed a variational ansatz assuming a Gaussian shape of the cloud (cf. [10]):

$$\psi_0 = N^{1/2}(2\pi)^{-3/4}(L_\rho^2 L_z)^{-1/2} e^{-\rho^2/4L_\rho^2} e^{-z^2/4L_z^2}. \quad (2)$$

Minimizing the energy functional  $H$  of the system, we found the aspect ratio of the cloud  $L$  and established that it decreases with increasing  $\sigma$  for  $l < l_*$ , and increases otherwise. The point  $l_*$  can be estimated by requiring  $dL/d\sigma|_{\sigma=0} = 0$ , which provides  $l_* = 0.41$  in good agreement with the numerical calculation.

At the critical point  $N = N_c$ , we observe that the local minimum of  $H$  becomes a saddle point. Hence, one has

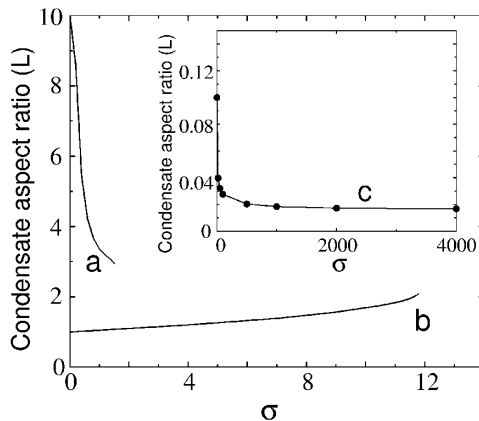


FIG. 3. Condensate aspect ratio  $L$  versus  $\sigma$  for (a)  $l = 10$ , (b)  $l = 1$ , and (in the inset) (c)  $l = 0.1$ . Curves (a) and (b) end when the system enters the unstable regime.

$(\partial^2 H / \partial L_z^2)(\partial^2 H / \partial L_\rho^2) - (\partial^2 H / \partial L_z \partial L_\rho)^2 = 0$ , in addition to  $\partial H / \partial L_z = \partial H / \partial L_\rho = 0$ . This gives the relation between  $L$  and  $l$  at the criticality,

$$\frac{(2L^2 + 1)(5 + 10l^4)}{2L^4 + 1} - \frac{6B(L)(1 + 2l^4)}{(L^2 - 1)^2} - 1 = 2 \frac{l^4}{L^2}, \quad (3)$$

where  $B(L) = 2 + L^2 - 3L \arctan[\sqrt{1 - L^2}/L] / \sqrt{1 - L^2}$ . Similarly, one can find the corresponding expressions for  $\sigma$ ,  $L_z$ , and  $L_\rho$  as a function of  $\omega_{z,\rho}$ . The result of Eq. (3) differs by less than 15% from our numerical calculations.

We have also analyzed the dynamics of the instability, evolving (in real time) the initially stable condensate by a slow increase of  $\sigma$ . In our approach based on the GPE, similar to the case of  $a < 0$  (see [12]), the dipolar condensate collapses to a point on a finite time scale. The ratio  $L$  increases moderately in the course of the collapse. The results for the spherical trap are presented in Fig. 4. The collapse in cigar-shaped traps occurs in a similar way, since the initial shape of the collapsing dipolar cloud is almost the same as in spherical traps (see Fig. 1).

As we see, the ground state of a dipolar gas exhibits a very rich behavior and one finds various BEC regimes. In order to electrically polarize an ultracold cloud of heteronuclear molecules, and thus create a molecular dipolar gas, one should have the electric field which provides the Stark potential  $dE$  greatly exceeding the spacing between the lowest rotational levels of the molecule. Then the rotational motion of the molecules will be “frozen” and their dipole moments will be oriented along the direction of the field. For most of the diatomic molecules the rotational level spacing is in the range from 0.1 to 1 K, and hence the required electric field is  $E \sim 10^3$  V/cm.

Molecular BEC is not yet achieved experimentally. We thus propose a method of inducing electric dipoles, which can be used in atomic condensates. The idea is to apply

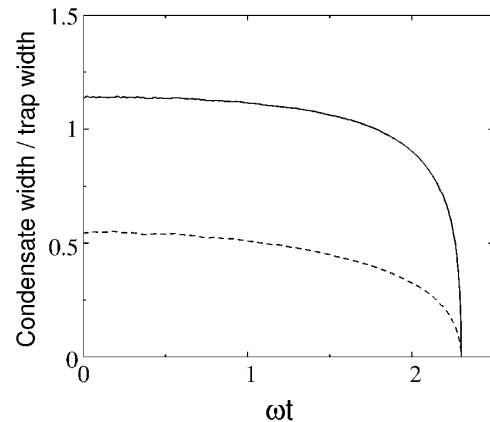


FIG. 4. Condensate widths (in units of  $a_z$ ) in the dipole direction (solid line) and perpendicular to the dipole (dashed line), for the collapse in a spherical trap of frequency  $\omega$  [ $\sigma(0) = 11.5 < \sigma_c = 11.8$ , and  $\sigma(t) = 11.5 + 0.8\omega t$ ].

a constant electric field and to optically admix the permanent dipole moment of a low-lying Rydberg state to the atomic ground state. Rydberg states of hydrogen and alkali atoms exhibit a linear Stark effect [13]: an electric field  $E_s$  splits the manifold of Rydberg states with given principal quantum number  $n$  and magnetic quantum number  $m$  into  $2(n - |m| - 1)$  Stark states. The outermost Stark states have permanent dipole moments  $d_R \sim n^2 e a_B$  (with  $a_B$  the Bohr radius), and there will be a related dipole-dipole force between the atoms.

This dipole-dipole interaction can be controlled with a laser [14]. This is achieved either by admixing the permanent dipole moment of the Stark states to the atomic ground state with an off-resonant cw laser, or by a stroboscopic excitation with a sequence of laser pulses. The pulses tuned to the lowest Stark state of a given Rydberg manifold should be separated by a time  $T$ , have duration  $2\Delta t \ll T$ , and have an area  $2\pi$  [15]. The field  $E_s$  and the “dressing” light have to be chosen such that they do not couple the selected lowest Stark state to other states, and the spacing ( $\sim n e a_B E_s$ ) between the adjacent Stark states should greatly exceed the mean-field dipole-dipole interaction in order to avoid the interaction-induced coupling. Stroboscopic excitation “dresses” the atomic internal states, so that each atom acquires a time averaged dipole moment of the order of  $d_s = n^2 e a_B f$ , oriented in the direction of  $E_s$ . Even though  $f = \Delta t/T$  is assumed to be small, the induced dipole can be rather large for  $n \gg 1$ . For  $\Delta t = 1$  ns,  $T = 10$   $\mu$ s, and  $n = 20$ , we obtain  $d_s = 0.1$  D. In the limit  $f \rightarrow 0$ ,  $n^2 f = \text{const}$ , the resulting time dependent Hamiltonian can be replaced by its time average, leading to Eq. (1) with  $d = d_s$ . A characteristic time scale in Eq. (1) is of order the inverse trap frequency  $\omega^{-1}$ . Hence, in our case the dynamics of the system is described by Eq. (1) with  $d = d_s$ , if the condition  $\Delta t, T \ll \omega^{-1}$  is satisfied. This has been tested numerically for  $\Delta t/T = 10^{-4}$ : We reproduced our previous results of the static GPE by solving explicitly Eq. (1) for the stroboscopic dressing of atoms, i.e., by setting  $d = d_s/f$  in the time intervals  $\Delta t$  and  $d = 0$  otherwise.

Aside from inducing permanent electric dipoles, the stroboscopic dressing of atoms will somewhat modify the trapping potential and the scattering length related to the van der Waals interatomic forces. The corresponding corrections will be proportional to the small parameter  $f$ . There will also be losses due to spontaneous emission and blackbody radiation [14]. The rates of these processes become comparable with each other for  $n = 20$  [13,14], where the corresponding decay time is of order 20  $\mu$ s. In our scheme the lifetime will be thus  $\approx 20 \mu\text{s}/f \approx 0.2$  s.

The laser resonant with a bare transition frequency dresses only the atoms that are sufficiently separated from their neighbors, since otherwise the dipole-dipole interaction shifts atomic resonances. Atomic pairs are “shielded” [16] and not dressed at interatomic distances smaller than  $R_*$ , where the latter follows from the equation  $\hbar\Omega \approx d_R^2/R_*^3$ , with  $\Omega = \pi/\Delta t$  being the Rabi frequency

associated with the dressing laser. For  $n = 20$  and  $\Delta t = 1$  ns we have  $\Omega = 500$  MHz and  $R_* = 0.7$   $\mu$ m.

The most dangerous “underwater stone” concerns inelastic decay processes. Fortunately, the “shielding” can suppress Penning ionization: a strong suppression is expected if atoms practically do not move during the short time  $\Delta t$ , and the distances at which the ionization occurs ( $\sim n^2 a_B$ ) are significantly smaller than  $R_*$ . For the parameters considered above this should be the case. The dipole-dipole interaction also induces the change of the effective Rabi frequency, and therefore the  $2\pi$  pulse condition is not strictly satisfied. Hence, a fraction of atoms remains in the Rydberg state between the stroboscopic pulses and decays due to spontaneous emission. This fraction can be reduced by decreasing the quantity  $\tilde{n} d^2 \Delta t$ , where  $\tilde{n}$  is the gas density. A detailed analysis of inelastic processes in the conditions of stroboscopic dressing of atoms requires a separate investigation.

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