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DOI
10.1103/PhysRevA.87.025601

Publication date
2013

Document Version
Final published version

Published in
Physical Review A

PHYSICAL REVIEW A **87**, 025601 (2013)

Two-dimensional dipolar Bose gas with the roton-maxon excitation spectrum

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(Received 14 December 2012; published 4 February 2013)

We discuss fluctuations in a dilute two-dimensional Bose-condensed dipolar gas, which has a roton-maxon character of the excitation spectrum. We calculate the density-density correlation function, fluctuation corrections to the chemical potential, compressibility, and normal (superfluid) fraction. It is shown that the presence of the roton strongly enhances fluctuations of the density, and we establish the validity criterion of the Bogoliubov approach. At $T = 0$ the condensate depletion becomes significant if the roton minimum is sufficiently close to 0. At finite temperatures exceeding the roton energy, the effect of thermal fluctuations is stronger and it may lead to a large normal fraction of the gas and compressibility.

DOI: 10.1103/PhysRevA.87.025601 PACS number(s): 03.75.Nt, 05.30.Jp

In the last decade, ultracold gases of dipolar particles, which include atoms with a large magnetic moment and polar molecules, have attracted a great deal of interest [1–4]. Being electrically or magnetically polarized, such particles interact with each other via long-range anisotropic dipole-dipole forces, which drastically changes the nature of quantum degenerate regimes. Experiments with chromium atoms (magnetic moment $6\mu_B$) [2], together with theoretical studies [5,6], have revealed the dependence of the shape and stability diagram of trapped dipolar Bose-Einstein condensates on the trapping geometry and interaction strength. They initiated spinor physics with quantum dipoles [7,8], and now dysprosium [9] and erbium [10] atoms (magnetic moments $10\mu_B$ and $7\mu_B$, respectively) have also entered the game. Recently, fascinating prospects for the observation of novel quantum phases have been opened by the creation of ultracold clouds of polar molecules and their cooling almost to quantum degeneracy [3,11]. In this case, the dipole-dipole forces can be orders of magnitude larger, and one has the possibility of manipulating the molecules by making use of their rotational degrees of freedom.

For dipolar Bose-condensed gases, one of the key issues was related to the presence of the roton-maxon character of the excitation spectrum and to the possibility of obtaining supersolid states in which the condensate wave function is the superposition of a uniform background and a lattice structure. The roton-maxon structure of the spectrum was first predicted for strongly pancaked Bose-Einstein condensates [12]. However, the idea of obtaining a supersolid state when the roton reaches 0 and the uniform BEC becomes unstable did not succeed because of the collapse of the system [13,14]. Since that time, several proposals have been made for the creation of supersolid states with bosons [15]. They rely on the potential of interatomic interaction which is flat at short distances and decays at large separations, and the results then indicate the presence of dense supersolid clusters [16].

This activity brought in analogies with liquid helium, where studies of the roton-maxon spectrum and attempts to observe the supersolid state experimentally have spanned decades [17,18] since the early theoretical prediction [19]. However, the most credible claim to observation of the supersolid [20] has now been withdrawn [21]. It is worth mentioning that the old idea of obtaining a stable density-modulated state (supersolid) in superfluid helium moving at a supercritical velocity [22] is now being discussed in the general context of superfluidity in Bose gases flowing with velocities higher than the Landau critical velocity [23].

The roton-maxon character of the excitation spectrum has also attracted great attention by itself. In relation to liquid helium, it has been discussed how the position of the roton minimum influences the phenomenon of superfluidity [18]. In the context of dipolar bosons in two dimensions, numerical calculations of the zero-temperature phase diagram [24–26] found that the reduction of the condensed fraction with an increase in density can be attributed to the appearance of the roton minimum. Finite-temperature Monte Carlo calculations [27] have revealed that the rotonization of the spectrum can decrease the Kosterlitz-Thouless superfluid transition temperature. Although the calculations [24–27] were focused on fairly high densities, they raised the question of the applicability of the Bogoliubov approach for dipolar bosons [26]. At the same time, there was extended activity on the static and dynamical properties of dilute trapped dipolar BECs on the basis of the Bogoliubov approach [28–31].

It is therefore instructive to identify the validity criterion of the Bogoliubov approach for Bose-condensed dipolar gases with the roton-maxon excitation spectrum, and this is the subject of the present paper. We show that at zero temperature the density fluctuations originating from the presence of the roton minimum lead to a significant depletion of the condensate and modify thermodynamic quantities if the roton minimum is sufficiently close to 0. At finite temperatures exceeding the roton energy, thermal density fluctuations may have a much stronger influence, leading to a large increase in the normal fraction and compressibility.

We consider a dilute Bose-condensed gas of dipolar bosons (tightly) confined in one direction (z) to zero-point oscillations and assume that in the x,y plane the translational motion is free (see Fig. 1). The dipole moments are oriented perpendicularly to the x,y plane, which, for electric dipoles (polar molecules), can be done by applying an electric field and, for magnetic atoms, by using a magnetic field. In this quasi-two-dimensional (2D) geometry, at large interparticle

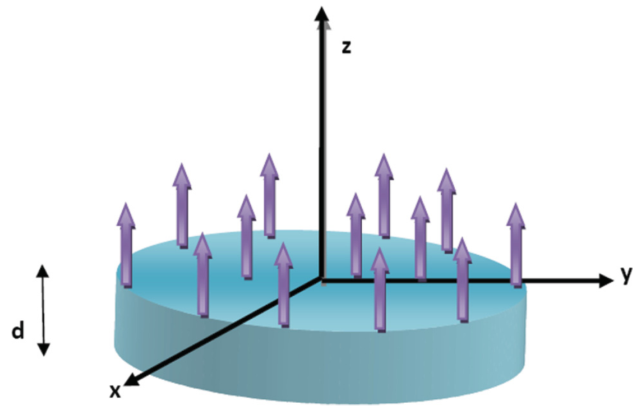

FIG. 1. (Color online) Dipolar Bose-Einstein condensate tightly confined in one direction.

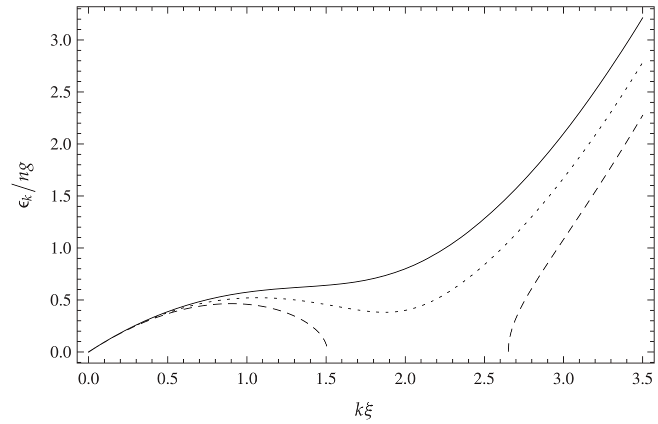

FIG. 2. Excitation energy ε_k of a quasi-2D dipolar BEC as a function of momentum k for several values of k_r. The solid curve ($k_r\xi = 1.84$) shows a monotonic dependence ε_k, the dotted curve ($k_r\xi = 1.96$) is ε_k with the roton-maxon structure, and the dashed curve ($k_r\xi = 2.08$) corresponds to a dynamically unstable BEC.

separations r the interaction potential is

$$V(r) = \frac{d^2}{r^3} = \frac{\hbar^2 r_*}{mr^3}, \tag{1}$$

with d being the dipole moment, m the particle mass, and $r_* = md^2/\hbar^2$ the characteristic dipole-dipole distance. The short-range part of the potential is assumed to be such that there is a roton-maxon excitation spectrum. In the ultracold limit where the particle momenta satisfy the inequality $kr_* \ll 1$, the off-shell scattering amplitude, defined as $f(\vec{k},\vec{k}') = \int \exp(-i\vec{k}'\cdot\vec{r}')V(r)\psi_{\vec{k}}(\vec{r})d^2r$ ($\psi_{\vec{k}}(\vec{r})$ is the wave function of the relative motion with momentum $\vec{k}$), is given by (see [32] and references therein):

$$f(\vec{k},\vec{k}') = \frac{\hbar^2}{m}\left[\frac{2\pi}{\ln(\kappa/k) + i\pi/2} - 2\pi r_*|\vec{k} - \vec{k}'|\right], \tag{2}$$

where we omit higher order terms in k. The second term on the right-hand side represents the so-called anomalous contribution coming from distances of the order of the de Broglie wavelength of particles [33]. It takes into account all partial waves and is obtained using a perturbative approach in $V(r)$. The first term on the right-hand side of Eq. (2) describes the short-range contribution. It is obtained by putting $k' = 0$ and proceeding along the lines of the 2D scattering theory [33]. The parameter κ depends on the behavior of $V(r)$ at short distances. In the quasi-2D geometry it also depends on the confinement length in the z direction, $l_0 = \sqrt{\hbar/m\omega_0}$, where ω_0 is the confinement frequency. One then can express κ through the 3D coupling constant g_{3D}. If the 3D s-wave scattering length, $a_{3\mathrm{D}} = mg_{3\mathrm{D}}/4\pi\hbar^2 \ll l_0$, then κ is exponentially small [34,35] and we may omit the k dependence under logarithm in Eq. (2), as well as $i\pi/2$ in the denominator of the first term. This gives $f(\vec{k},\vec{k}') = g(1 - C|\vec{k} - \vec{k}'|)$, where the 2D short-range coupling constant is $g = g_{3\mathrm{D}}/\sqrt{2}l_0$ and $C = 2\pi\hbar^2 r_*/mg = 2\pi d^2/g$. Employing this result in the secondly quantized Hamiltonian [13,14], we obtain

$$\hat{H} = \sum_{\vec{k}} E_k \hat{a}^\dagger_{\vec{k}}\hat{a}_{\vec{k}} + \frac{g}{2S}\sum_{\vec{k},\vec{q},\vec{p}}(1 - C|\vec{q} - \vec{p}|)\hat{a}^\dagger_{\vec{k}+\vec{q}}\hat{a}^\dagger_{\vec{k}-\vec{q}}\hat{a}_{\vec{k}+\vec{p}}\hat{a}_{\vec{k}-\vec{p}}, \tag{3}$$

where S is the surface area, $E_k = \hbar^2k^2/2m$, and $\hat{a}^\dagger_{\mathbf{k}}$ and $\hat{a}_{\mathbf{k}}$ are the creation and annihilation operators of particles. At zero temperature there is a true BEC in two dimensions, and we may use the standard Bogoliubov approach. Assuming the weakly interacting regime where $mg/2\pi\hbar^2 \ll 1$ and $r_* \ll \xi$, with $\xi = \hbar/\sqrt{mng}$ being the healing length, we reduce Hamiltonian (3) to a bilinear form, use the Bogoliubov transformation $\hat{a}^\dagger_{\vec{k}} = u_k\hat{b}^\dagger_{\vec{k}} - v_k\hat{b}_{-\vec{k}}$, and obtain the diagonal form $\hat{H} = E_0 + \sum_{\vec{k}}\varepsilon_k\hat{b}^\dagger_{\vec{k}}\hat{b}_{\vec{k}}$ in terms of operators $\hat{b}^\dagger_{\vec{k}}$ and $\hat{b}_{\vec{k}}$ of elementary excitations. The Bogoliubov functions u_k and v_k are expressed in a standard way, $u_k,v_k = (\sqrt{\varepsilon_k/E_k} \pm \sqrt{E_k/\varepsilon_k})/2$, and the Bogoluibov excitation energy is given by $\varepsilon_k = \sqrt{E_k^2 + 2ngE_k(1 - Ck)}$.

To zero order the chemical potential is $\mu = ng$. For small momenta the excitations are sound waves, $\varepsilon_k = \sqrt{ng/mk}$. The dependence of ε_k on k remains monotonic with increasing k if $C \leqslant \sqrt{8}\xi/3$ (see Fig. 2). For the constant C in the interval

$$\frac{\sqrt{8}}{3}\xi \leqslant C \leqslant \xi, \tag{4}$$

the excitation spectrum has a roton-maxon structure. It is then convenient to represent ε_k in the form

$$\varepsilon_k = \frac{\hbar^2 k}{2m}\sqrt{(k - k_r)^2 + k_\Delta^2}, \tag{5}$$

where $k_r = 2C/\xi^2$ and $k_\Delta = \sqrt{4/\xi^2 - k_r^2}$. If the roton is close to 0, then k_r is the position of the roton, and

$$\Delta = \hbar^2 k_r k_\Delta/2m = 2ngC\sqrt{mng/\hbar^2 - C^2(mng/\hbar^2)^2} \tag{6}$$

is the height of the roton minimum (see Fig. 2). For $C = \xi$ the roton minimum touches 0, and at larger C the uniform Bose condensate becomes dynamically unstable.

It should be noted that the coupling constant g can be tuned by using Feshbach resonances or by modifying the frequency of the tight confinement ω_0. Therefore, although the range of C given by Eq. (4) is rather narrow, it can be reached without serious difficulties. The condition $C = 2\pi d^2/g = \xi$ is reduced to $(mg/2\pi\hbar^2) = a_{3\mathrm{D}}/\sqrt{2}l_0 \simeq 2\pi nr_*^2$. For dysprosium atoms we have the dipole-dipole distance $r_* \simeq 200$ Å, and at 2D densities $\sim 10^9$ cm^{-2} the roton-maxon spectrum is realized for the 3D scattering length a_{3D} of several tens of angstroms at the frequency of the tight confinement of 10 kHz, leading to a confinement length l_0 of about 1000 Å.

The Bogoliubov approach assumes that the density and phase fluctuations are small. In the 2D case at $T = 0$, the presence of the roton does not significantly change the phase fluctuations and they remain small. However, the situation with density fluctuations is different. Writing the operator of the density fluctuations as (see [36]) $\delta\hat{n} = \sqrt{n}\sum_{\vec{k}}(u_k - v_k)\exp(i\vec{k}\cdot\vec{r})\hat{b}_{\vec{k}} + \text{H.c.}$, we obtain for the density-density correlation function:

$$\frac{\langle\delta\hat{n}(\vec{r})\delta\hat{(0)}\rangle}{n^2} = \frac{1}{n}\int\frac{d^2k}{(2\pi)^2}\frac{E_k}{\varepsilon_k}(1+2N_k)\exp(i\vec{k}\cdot\vec{r}), \quad (7)$$

where $N_k = [\exp(\varepsilon_k/T) - 1]^{-1}$ are occupation numbers for the excitations. It is instructive to single out the roton contribution to the correlation function, (7). Asuming that the roton is close to 0 and the roton energy is $\Delta \ll ng$, we have the coefficient C close to ξ, and $k_r \simeq 2/\xi$. Then, using Eqs. (5) and (7), for the contribution of momenta near the roton minimum at, $T = 0$ we obtain

$$\frac{\langle\delta\hat{n}(\mathbf{r})\delta\hat{n}(0)\rangle_r}{n^2} = \frac{2mg}{\pi\hbar^2}\ln\left(\frac{2ng}{\Delta}\right)J_0(2r/\xi); \quad \Delta \ll ng, \quad (8)$$

where J_0 is the Bessel function.

We thus see that the density fluctuations grow logarithmically when the roton minimum is approaching 0 and they can become strong for very small Δ. In this case they lead to a significant depletion of the condensate. The noncondensed density of particles is $n' = \int v_k^2 d^2k/(2\pi)^2$ and the integral over dk is logarithmically divergent at large momenta because of the dipolar contribution to the interaction strength, $-gCk$. However, this form of the dipole-dipole contribution is valid only for $k \ll 1/r_*$. We thus may set a high momentum cut-off, $1/r_*$, which leads to (see Fig. 3)

$$\frac{n'}{n} = \frac{mg}{4\pi\hbar^2}\left[1 - k_r\xi - \frac{3(k_r\xi)^2}{4} + \frac{(k_r\xi)^2}{2}\ln\left(\frac{\xi}{r_*(2-k_r\xi)}\right)\right]. \quad (9)$$

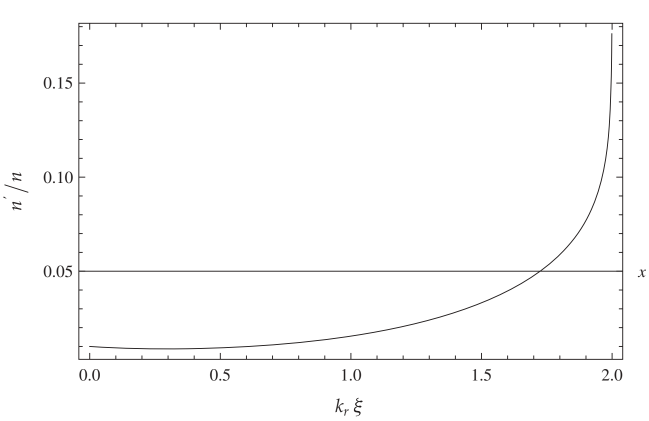

FIG. 3. Noncondensed fraction as a function of $k_r\xi$ for $mg/4\pi\hbar^2 = 0.01$ ($\xi/r_* = 100/k_r\xi$). A similar increase in the noncondensed fraction with decreasing roton energy Δ was found in numerical calculations in Ref. [28].

In the absence of the dipole-dipole interaction ($r_* = 0$ and $k_r = 0$) we recover the usual result for the 2D BEC with short-range interparticle repulsion, $n' = n(mg/4\pi\hbar^2)$. For $\Delta \ll ng$ we have $(2 - k_r\xi) \simeq (k_\Delta\xi)^2/4$ and Eq. (9) transforms to

$$\frac{n'}{n} \simeq \frac{mg}{\pi\hbar^2}\ln\left(\frac{2ng}{\Delta}\zeta\right), \quad \Delta \ll ng, \quad (10)$$

where $\zeta = \sqrt{2\pi\hbar^2/e^2mg}$.

As we see from Eqs. (8) and (10), for a roton minimum close to 0 a small condensate depletion and small fluctuations of the density require the inequality $(mg/\pi\hbar^2)\ln(2ng/\Delta) \ll 1$. It differs only by a logarithmic factor $\ln(2ng/\Delta)$ from the small parameter of the theory, $(mg/2\pi\hbar^2) \ll 1$, in the absence of a roton. The same logarithmic factor appears in the fluctuation correction to the chemical potential and in the one-body density matrix $g_1(r) = \langle\hat{\Psi}^\dagger(\vec{r})\hat{\Psi}(0)\rangle$, where $\hat{\Psi}(\vec{r})$ is the field operator. Assuming that the roton minimum is close to 0 and taking into account only the contribution of momenta near this minimum, for $\Delta \ll ng$ we have

$$g_1(r) = n_0\left[1 + \frac{mg}{\pi\hbar^2}\ln\left(\frac{2ng}{\Delta}\right)J_0(2r/\xi)\right]. \quad (11)$$

The correction to the chemical potential due to quantum fluctuations is given by

$$\frac{\delta\mu}{\mu} \simeq \frac{2mg}{\pi\hbar^2}\ln\left(\frac{2ng}{\Delta}\right), \quad \Delta \ll ng. \quad (12)$$

However, the situation changes in the calculation of the compressibility. At $T = 0$ the inverse compressibility is equal to $n^2\partial\mu/\partial n$. Then, using Eqs. (12) and (6), for a roton minimum close to 0, at $\Delta \ll ng$ we obtain

$$\frac{\partial\mu}{\partial n} = g\left[1 + \frac{2mg}{\pi\hbar^2}\ln\left(\frac{2ng}{\Delta}\right) + \frac{mg}{\pi\hbar^2}\left(\frac{2ng}{\Delta}\right)^2\right], \quad (13)$$

where g is the mean-field contribution, and the second and third terms originate from quantum fluctuations. Small deviations of the compressibility from the mean-field result require the inequality

$$\frac{mg}{\pi\hbar^2}\left(\frac{2ng}{\Delta}\right)^2 \ll 1. \quad (14)$$

We thus conclude that at $T = 0$ the validity of the Bogoliubov approach is guaranteed by the presence of the small parameter, (14). For the dysprosium example given after Eq. (6) we have $ng \sim 5$ nK, and criterion (14) is satisfied for a roton energy above 2 nK.

In two dimensions at finite temperatures, long-wave fluctuations of the phase destroy the condensate [37–39]. There is the so-called quasicondensate, or condensate with fluctuating phase. In this state fluctuations of the density are suppressed but the phase still fluctuates. The transition from a noncondensed state to a quasi-BEC is of the Kosterlitz-Thouless type and it occurs through the formation of bound vortex-antivortex pairs [40]. Somewhat below the Kosterlitz-Thouless transition temperature the vortices are no longer important, and in the weakly interacting regime that we consider the phase coherence the length l_ϕ is exponentially large. Thermodynamic properties, excitations, and correlation properties on a distance scale smaller than l_ϕ are the same as in the case of a true BEC. Moreover, for realistic parameters of quantum gases, l_ϕ exceeds the size of the system [41], so that one can employ the ordinary BEC theory.

Irrespective of the relation between l_ϕ and the size of the system, one may act in terms of the density and phase variables (hydrodynamic approach). We now show that the rotonization of the spectrum can strongly increase thermal fluctuations of the density and destroy the Bose-condensed state even at very low T. Using Eq. (7) we calculate the density-density correlation function. Assuming that the roton energy Δ is very low (at least $\Delta \ll T$), the main contribution to the integral in Eq. (7) comes from momenta near k_r, and we obtain

$$\frac{\langle \delta\hat{n}(\mathbf{r})\delta\hat{(0)}\rangle}{n^2} = \frac{4mg}{\hbar^2}\frac{T}{\Delta}J_0(2r/\xi), \tag{15}$$

where it is also assumed that $k_\Delta r \ll 1$. Comparing this result with Eq. (8) we see that instead of the logarithmic factor we have $2\pi T/\Delta \gg 1$.

The same factor appears in the correction to the chemical potential due to thermal fluctuations:

$$\frac{\delta\mu}{\mu} = \sum_{\mathbf{k}}(u_k - v_k)^2 N_k \simeq \frac{2mg}{\hbar^2}\frac{T}{\Delta}, \quad \Delta \ll T. \tag{16}$$

We now calculate the density of the normal component in the presence of the roton. In two dimensions the expression for this quantity reads (cf. [36])

$$n_T = -\int \frac{\hbar^2 k^2}{2m}\frac{\partial N_k}{\partial \varepsilon_k}\frac{d^2k}{(2\pi)^2}.$$

If the roton minimum is close to 0 and $\Delta \ll T$, then the momenta near the roton minimum are the most important, and the integration over dk yields

$$\frac{n_T}{n} = \frac{2mg}{\hbar^2}\frac{T}{\Delta}. \tag{17}$$

The employed approach requires the condition $n_T \ll n$ because we used the spectrum of excitations obtained by the Bogoliubov method. Again, at temperatures $T \gtrsim \Delta$ we should have the inequality $(2mg/\hbar^2)T/\Delta \ll 1$.

A different small parameter appears in the calculation of the compressibility. The inverse isothermal compressibility is proportional to $(\partial P/\partial n)_T$, where the pressure is $P = -(\partial F/\partial S)_T$, with the free energy given by $F = E_0 + T\sum_{\mathbf{k}} \ln[1 - \exp(-\varepsilon_k/T)]$. For a roton minimum close to 0 and $\{T, ng\} \gg \Delta$, we obtain

$$\left(\frac{\partial P}{\partial n}\right)_T = ng\left[1 - \frac{mg}{\hbar^2}\left(\frac{2ng}{\Delta}\right)^2\frac{T}{\Delta} + \cdots\right], \tag{18}$$

where we omitted less important finite-temperature contributions and the zero-temperature contribution proportional to the small parameter, (14). Equation (18) shows that at $T \gg \Delta$ the Bogoliubov approach requires the inequality

$$\frac{mg}{\hbar^2}\left(\frac{2ng}{\Delta}\right)^2\frac{T}{\Delta} \ll 1, \tag{19}$$

whereas for $T \lesssim \Delta$ it is sufficient to have criterion (14).

For certain quantities the Bogoliubov approach may give good results at $T \gg \Delta$ if $(mg/\hbar^2)T/\Delta \ll 1$ and at $T \lesssim \Delta$ in the presence of the ordinary small parameter $mg/2\pi\hbar^2$ amplified by a logarithmic factor $\ln(2ng/\Delta)$ for $ng \gg \Delta$. However, the validity of this approach is guaranteed only if inequalities (19) and (14) are satisfied. For $T \gg \Delta$ the compressibility following from Eq. (18) and the normal fraction given by Eq. (17) can become significant, by far exceeding similar quantities in an ordinary 2D Bose gas with short-range interactions at the same temperature, coupling constant g, and density.

In conclusion, we have shown that the roton-maxon structure of the excitation spectrum, which can be achieved in dipolar Bose-condensed gases in 2D geometry, strongly enhances the density fluctuations. We obtained the validity criterion of the Bogoliubov approach and found that at finite temperatures in the dilute regime where $nr_*^2 \ll 1$, thermal fluctuations may significantly increase the compressibility and reduce the superfluid fraction even at temperatures well below the Kosterlitz-Thouless transition temperature.

We are grateful to L. P. Pitaevskii and D. S. Petrov for stimulating discussions. We acknowledge support from CNRS, from the University of Chlef, and from the Dutch Foundation FOM.

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