Supersolid edge and bulk phases of a dipolar quantum gas in a box

S. M. Roccuzzo, S. Stringari, and A. Recati
INO-CNR BEC Center and Dipartimento di Fisica,
Università degli Studi di Trento, 38123 Povo, Italy and
Trento Institute for Fundamental Physics and Applications, INFN, 38123, Trento, Italy

(Dated: June 29, 2021)

We investigate the novel density distributions acquired by a dipolar Bose-Einstein condensed gas confined in a box potential, with special focus on the effects of supersolidity. Differently from the case of harmonic trapping, the ground state density reveals a strong depletion in the bulk region and an accumulation of atoms near the walls, well separated from the bulk, as a consequence of the competition between the attractive and the repulsive nature of the dipolar force. In a quasi two-dimensional geometry characterized by cylindrical box trapping, we observe the emergence of a ring-like configuration near the boundary of the box, revealing peculiar supersolid and crystal effects in a useful range of parameters. In the case of square box trapping the density oscillations along the edges, caused by the enhanced accumulation of atoms near the vertices, exhibit interesting analogies with the case of box trapped one dimensional configurations. For sufficiently large values of the atom number also the bulk region can exhibit supersolidity, the resulting geometry reflecting the symmetry of the confining potential even for large systems.

Introduction. Bose-Einstein condensed atomic gases have proved to be an invaluable tool for the study of the physics of many body systems. However, while typical many body problems consider translationally invariant systems in the thermodynamic limit, Bose-Einstein condensates (BECs) are ordinarily realized in small, inhomogeneous samples confined by harmonic potentials [1]. Although harmonic trapping allows the study of relevant properties of these many body systems (e.g. collective excitations [2] [3], superfluid properties [4] [6], quantized vortices [7] [9]), other important properties, like sound propagation or critical behaviors, can be better studied in uniform systems. For these reasons, Bose-Einstein condensation in “box” potentials has been an emerging topic of research in recent years, leading to the realization of uniform BECs in gases of alkali atoms and first important measurements in both 3D and 2D configurations [10] [17].

The achievement of BECs of magnetic atoms in harmonic traps [15] [21] opened the way to the study of the very peculiar phenomena, which includes a geometry dependence of the phase diagram stability [22], a rotonized excitation spectrum [23] [26], quantum droplets [27] [30] and more recently supersolidity [31] [36]. While most of the theories for supersolidity are developed for infinite systems, for uniformly confined systems all the experiments have been so far conducted in harmonic traps.

The natural question which arises is therefore how a dipolar gas behaves in a box potential, and to what extent its configurations mimic their thermodynamic counterparts. First theoretical investigations carried out in the deep superfluid phase [37] have pointed out the peculiar phenomenon of accumulation of the density distribution near the boundary, as a consequence of the repulsive behavior of the aligned dipoles. This effect is strongly reduced in the presence of transverse harmonic trapping because of the high energetic cost for dipoles to move away from the center of the trap. The present work is based on a proper generalization of the Gross-Pitaevskii equation which contains the terms due to the Lee-Huang-Yang (LHY) correction to the mean field equation of state and it mainly focuses on the new supersolid features exhibited by the system in the presence of the box. We find that in two-dimensional geometries the accumulation along the border is enhanced in the regimes where the LHY correction is relevant, creating edges pretty well separated from the bulk. For a relatively small number of atoms, the bulk remains in a low density superfluid phase, while the edges can show typical supersolid or droplet crystal structures (see Fig. 1). Increasing the atom density leads to a supersolid bulk region, while the edges can be found to be in a high-density superfluid phase (see Fig. 4). Moreover, the lattice emerging in the bulk has not in general a triangular (or honeycomb) pattern, as expected for an infinite system [38], but its structure is dictated by the shape of the confining box potential even for relatively large systems.

The Model. We start our exploration by considering the case of a quasi 2-dimensional dipolar BEC, obtained by imposing a harmonic confinement only in the polarization direction (z-axis). At zero temperature, the dipolar BEC is described by a macroscopic wave function \( \Psi(\mathbf{r}, t) \), whose square modulus gives the local density of the system, and which obeys to the so-called extended Gross-Pitaevskii equation (eGPE) [39] [40]

\[
\begin{align*}
\mathcal{i}\hbar \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} &= \left[ -\frac{\hbar^2 \nabla^2}{2m} + V_{\text{ext}}(\mathbf{r}) + g |\Psi(\mathbf{r}, t)|^2 
+ \int d\mathbf{r}' V_{dd}(\mathbf{r} - \mathbf{r}') |\Psi(\mathbf{r}', t)|^2 + \gamma (\epsilon_{dd}) |\Psi(\mathbf{r}, t)|^3 \right] \Psi(\mathbf{r}, t) 
\end{align*}
\]

(1)

where \( V_{\text{ext}}(\mathbf{r}) \) is the trapping potential, \( g = 4\pi\hbar^2 a/m \) is the coupling constant fixed by the s-wave scattering length \( a \), \( V_{dd}(\mathbf{r}) = \frac{\mu a^2}{4\pi} \frac{1-3\cos^2 \theta}{|\mathbf{r}|^3} \) is the dipole-dipole
FIG. 1. Ground state integrated density profiles $n(x,y) = \int dz |\Psi(x,y,z)|^2$ for a gas of $10^5$ atoms of $^{164}$Dy confined in the polarization direction by a harmonic potential of frequency $\omega_z = (2\pi)100$Hz, and by a box potential in the x-y plane, with the shape of a circle of radius $R=10.185 \mu$m. The value of $\epsilon_{dd}$ for panels a), b) and c) is, respectively, 1.32, 1.404 and 1.467. The height of the box is fixed to $V_0 = 100\hbar \omega_z$

interaction between two identical magnetic dipoles $\mu$ aligned along the z-axis ($\theta$ is the angle between $\mathbf{r}$ and the z axis). A key dimensionless parameter is $\epsilon_{dd}$, defined as

$$\epsilon_{dd} = \frac{\mu_0 \mu^2}{3g}$$

which measures the relative strength of the dipolar and the contact interaction. Experimentally, the parameter $\epsilon_{dd}$ is tuned by changing the value of the s-wave scattering length $a$, thanks to the occurrence of a Feshbach resonance. The last term in the eGPE equation is the local density approximation of the Lee-Huang-Yang correction to the ground state energy of the system [30-40], with

$$\gamma(\epsilon_{dd}) = \frac{16}{3\sqrt{\pi}} g a^3 \text{Re} \left[ \int_0^\pi d\theta \sin(\theta) [1 + \epsilon_{dd}(3 \cos^2 \theta - 1)]^\frac{3}{2} \right].$$

The eGPE Eq. [4] provides a reliable description of the available experimental phenomenology. In the absence of confinement in the transverse direction, this model predicts, that for a certain value of the density and of $\epsilon_{dd}$, a phase transition between a uniform superfluid and a supersolid occurs. In the thermodynamic limit, the supersolid lattice is predicted to be triangular or honeycomb [38]. The occurrence of such lattice symmetry has been also predicted for the case of transverse, radially symmetric, harmonic trapping [32-41]. Very recently, the possible existence of other exotic configurations in harmonic traps has been proposed [42-43].

Circular box potential. We first consider the case where the transverse confinement in the x-y plane is provided by a circular box, while the confinement along the polarization direction (z-axis) is of harmonic nature. The case of a square box in the x-y plane will be discussed later, while the properties of a one-dimensional box will be discussed in the Supplementary Materials. We always fix the height of the box potential to a value large enough to ensure that the density goes practically to zero at the border. Similar configurations have been already experimentally realized to trap alkali atoms [13-15]. In Fig. 1 we show examples of the ground state density profiles (obtained by propagating equation 4 in imaginary time) of $N = 10^5$ atoms of $^{164}$Dy, for different values of $\epsilon_{dd}$. As already anticipated, most of the atoms accumulate at the edge of the confining potential, forming a quasi-one-dimensional ring structure well separated from the atoms in the bulk. For small values of $\epsilon_{dd}$ both the edge and the bulk remain in the superfluid phase, while increasing $\epsilon_{dd}$ (i.e. increasing the effect of the dipolar force), the edge region clearly undergoes a phase transition to the supersolid phase, where the density peaks near the boundary of the box exhibit a finite overlap, ensuring global phase coherence. The overlap between the density peaks disappears for even larger values of $\epsilon_{dd}$, the system forming a sort of one dimensional ring crystal.

The emergent edge ring geometry allows to estimate the superfluid density in terms of the Leggett variational expression [44-45]. To this purpose we write the ground-state density in cylindrical coordinates $\rho(\rho, \theta, z)$, so that the Leggett’s estimate for the superfluid density can be written as

$$\frac{n_S}{n} = \frac{2\pi}{n} \left( \int dr dz \rho(\rho, \theta, z) \right)^{-1}$$

where the integration over the radial coordinate is performed only in the edge region, identified by the density minima that appears both at the border of the box (where the density goes to zero), and at the interface between the edge and the bulk. In the case of the (extended) Gross-Pitaevskii equation the estimate [4] for the superfluid density has been already verified to coincide with the result obtained by imposing the twisted boundary condition to a one-dimensional array of droplets [46]. Remarkably in [47] it has been shown that Leggett’s estimate coincides with the exact superfluid density also in the case of peculiar stationary nonground state solutions (coidal wave solution) which exhibit a periodic density modulation. The estimate [4] reported in Fig. 2 (blue squares), reveals a critical dependence on $\epsilon_{dd}$, emphasizing the emergence of a phase transition between the superfluid and the supersolid phase at $\epsilon_{dd} = 1.4$ and a transition between the supersolid and the crystal phase, characterized by the vanishing of $n_S$, at $\epsilon_{dd} = 1.55$. These values are very close to the critical values calculated for one dimensional tubular configurations imposing periodic boundary conditions [24], after taking into account that in the edge configuration discussed here the number of atoms occupying the ring increases with $\epsilon_{dd}$, as shown in the same figure (red circles). Such an increase is actually particularly important in the supersolid phase as a consequence of the reduced value of the chemical potential, which favors the accumulation...
of dipoles on the density peaks, where the inter-atomic dipolar interaction is mainly attractive.

The novel configuration emerging in the box of circular shape discussed above is particularly attractive because in this case the boundary does not depend on the azimuthal coordinate and takes the form of a ring, where the dipolar particles form a one-dimensional structure, well separated from the atoms in the bulk. This provides the interesting possibility of exploring superfluid and supersolid features in uniform one-dimensional like configurations with periodic boundary conditions.

Square box potential. It is interesting to consider other forms of boxes like, for example, the most familiar square box. This case was considered in \cite{37} in the deep superfluid phase and in the absence of beyond-mean-field effects. Here, we consider also regimes where the mean field approach would yield instability and the LHY correction allows for the emergence of the supersolid and crystal phases.

The results for the density profiles in the case of a 2D square box are reported in Fig. 3 and reveal the same mechanism of accumulation of the density near the boundary already discussed in the case of a circular box. A major difference concerns the behavior of the density profile along the edge of the box. In fact the vertices of the square box become points of strong accumulation of dipoles, causing density modulations along the sides of the square, even for small values of $\epsilon_{dd}$ (see Fig. 3 panel a), when the system is in the superfluid phase. The behavior of the density along each edge of the square configuration shares interesting analogies with the behavior exhibited by a quasi one-dimensional gas confined by a box potential (see Supplementary Materials).

The above discussion reveals that the presence of the square box makes the identification of the transition between the superfluid, supersolid and crystal phases of the dipolar gas on the edge of the box more difficult than in the case of the circular box.

Bulk supersolidity. The configurations discussed so far do not reveal the emergence of supersolid effects in the bulk region, because of the small value of the bulk density caused by the accumulation of dipoles near the boundary. In order to observe the bulk supersolidity one consequently needs to increase significantly the atom density, in such a way that the density in the central region remains large enough to ensure the appearance of a crystal quantum phase. In Fig. 4 we have considered config-
urations containing \( N = 2 \times 10^6 \) atoms confined by a box potential in the transverse direction, with the shape of regular polygons (panels a-d) or circular (panel e), all with the same area (and hence the same number of atoms per unit surface). For the same value of \( \epsilon_{\text{dd}} = 1.36 \), these configurations exhibit a supersolid structure in the bulk, characterized by the typical overlap between neighbouring density peaks, well separated from the edge region by a density dip. Despite the number of atoms and system size considered, resulting in a large number of droplets (\( \approx 60 \)), the symmetry of the supersolid lattice reflects the one of the confining potential, implying that surface effects hinder the possibility of reaching the thermodynamic limit, where the lattice is expected to be triangular or honeycomb [5]. This can be qualitatively understood as a consequence of the long-range nature of the dipolar force and the formation of the edge. In fact, since the dipoles are in a mainly repulsive configuration, they tend to expand towards the edge, where they acquire a density profile with the same shape of the confining potential; the droplets that form in the bulk also tend to repel each other, but their expansion is stopped by the repulsion of the edge, so that they are forced to arrange in lines parallel to the sides of the edge. This behaviour is suppressed in an infinite system or in a harmonic trap, where the expansion of the gas is energetically unfavourable.

It is worth noticing that the supersolid and crystal structures at the edge of the boundary, which are well visible in the configurations of Fig. 1 and 3 (panels b and c), have disappeared in Fig. 4 as a consequence of the high density acquired by the system near the boundary, caused by the large value of \( N \). As pointed out in [18] and discussed also in [22], the density dependence of the critical value of the interaction parameter \( \epsilon_{\text{dd}}, \) which separates the superfluid from the supersolid phase, actually exhibits a characteristic non monotonic dependence (see also Fig. 5 in the Supplementary Materials). This implies that, for a properly fixed value of \( \epsilon_{\text{dd}}, \) if one increases the density starting from small values, the system undergoes first a phase transition from the superfluid to the supersolid (and eventually to the crystal) phase characterized by typical density oscillations, to come back again to the uniform superfluid phase at larger densities. Notice that this effect can also be observed with a smaller number of atoms, by confining the atoms in properly designed box potentials of smaller dimension. In fact, such density, although relatively high (\( \approx 10^{15} \text{ cm}^{-3} \) for the edge configurations shown in Fig. 3), is still compatible with the usual stability conditions imposed by three-body recombination, suggesting the possibility of observing this effect in actual experiments.

We have finally checked that the results presented in this work do not qualitatively change for different choices of the parameters. In particular we have considered different values of the transverse confinement in the interval \((2\pi)50\text{Hz} < \omega_y = \omega_z < (2\pi)150\text{Hz},\) and of system size and number of atoms. The actual choice of \( \omega_{y,z} \) can however affect the value of the density in the central region, the critical value of \( \epsilon_{\text{dd}} \) for the superfluid-supersolid phase transition, as well as the number of droplets which form in the supersolid phase, their relative distance being sensitive to the value of \( \omega_z \) [23].

In conclusion, we have investigated the ground state configurations of a dipolar Bose-Einstein condensed gas confined by a box potential. We have shown that the tendency of the density to accumulate near the walls, as a consequence of the repulsion between aligned dipoles, favours the formation of novel quasi-1d configurations located at the edge of the box and well separated from the atoms filling the bulk region. In the case of quasi-2d boxes of circular shape the edge configuration takes the characteristic form of a ring, revealing clear supersolid and crystal effects in a useful range of parameters. We have also shown that the geometry of the supersolid in the bulk region reflects the shape of the confining potential even for very large systems, therefore hindering the possibility of reaching the thermodynamic limit of dipolar BEC’s using box potentials. Natural extension of this work concern the study of the non equilibrium behavior exhibited by dipolar gases in the novel ring configuration formed at the edge of the circular box.

Acknowledgement Useful discussions with G. Modugno and the members of the Firenze-Pisa dipolar group are acknowledged. This project has received funding from Provincia Autonoma di Trento, the Q@TN initiative and the FISh project of the Istituto Nazionale di Fisica Nucleare, and the Italian MIUR under the PRIN2017 project CEnTraL.

[1] L. Pitaevskii and S. Stringari, Bose-Einstein condensation and superfluidity (Oxford University Press, 2016).
[2] S. Stringari, Phys. Rev. Lett. 77, 2360 (1996).
[3] M.-O. Mewes, M. R. Andrews, N. J. van Druten, D. M. Kurn, D. S. Durfee, C. G. Townsend, and W. Ketterle, Phys. Rev. Lett. 77, 988 (1996).
[4] D. Guéry-Odelin and S. Stringari, Phys. Rev. Lett. 83, 4452 (1999).
[5] O. M. Maragò, S. A. Hopkins, J. Arlt, E. Hodby, G. Hechenblaikner, and C. J. Foot, Phys. Rev. Lett. 84, 2056 (2000).
[6] C. D. Rossì, R. Dubessy, K. Merloti, M. de Goër de Herve, T. Badr, A. Perrin, L. Longchambon, and H. Perrin, New Journal of Physics 18, 062001 (2016).
[7] K. W. Madison, F. Chevy, W. Wohlleben, and J. Dalibard, Phys. Rev. Lett. 84, 806 (2000).
[8] J. R. Abo-Shaeer, C. Raman, J. M. Vogels, and W. Ketterle, Science 292, 476 (2001).
[9] L. Pitaevskii and S. Stringari, Bose-Einstein condensation and superfluidity (Oxford University Press, 2016).
[10] S. Stringari, Phys. Rev. Lett. 77, 2360 (1996).
[11] M.-O. Mewes, M. R. Andrews, N. J. van Druten, D. M. Kurn, D. S. Durfee, C. G. Townsend, and W. Ketterle, Phys. Rev. Lett. 77, 988 (1996).
[12] D. Guéry-Odelin and S. Stringari, Phys. Rev. Lett. 83, 4452 (1999).
[13] O. M. Maragò, S. A. Hopkins, J. Arlt, E. Hodby, G. Hechenblaikner, and C. J. Foot, Phys. Rev. Lett. 84, 2056 (2000).
[14] C. D. Rossì, R. Dubessy, K. Merloti, M. de Goër de Herve, T. Badr, A. Perrin, L. Longchambon, and H. Perrin, New Journal of Physics 18, 062001 (2016).
[15] K. W. Madison, F. Chevy, W. Wohlleben, and J. Dalibard, Phys. Rev. Lett. 84, 806 (2000).
[16] J. R. Abo-Shaeer, C. Raman, J. M. Vogels, and W. Ketterle, Science 292, 476 (2001).
[17] https://science.sciencemag.org/content/292/5516/476.full.pdf
A. Quasi one-dimensional dipolar Bose gas in a box

To complement our analysis of the behavior of a dipolar Bose gas in presence of hard walls, we have also considered the case of a quasi-one-dimensional configuration confined by a box potential in the elongated direction. We have in particular determined the ground-state density profiles of $N = 4 \times 10^4$ atoms of $^{164}$Dy confined in a trapping potential of the form $V_{\text{ext}} = \frac{1}{2}m(\omega_x^2 y^2 + \omega_z^2 z^2) + V_{\text{box}}(x, L)$, with $\omega_y = \omega_z = (2\pi)100\text{Hz}$, $V_{\text{box}}(x, L) = V_0$ for $|x| \geq L$ and 0 otherwise, $V_0 = 100\hbar\omega_z$ and $L=12\mu m$. Typical density profiles for different values of $\epsilon_{dd}$ are reported in Fig. 5a,b,c. The profiles reported in panels a,d (respectively, b,e and c,f) are calculated by fixing $\epsilon_{dd}=1.32$ (respectively, 1.39 and 1.46) and e) correspond to a superfluid phase. The configuration d) and f) corresponde to a superfluid phase. The configuration c) is characterised by a pronounced roton minimum, precursor of the instability to a periodically modulated density (supersolid phase) for larger values of $\epsilon_{dd}$ (panel f)). In the presence of the box atoms accumulate close to the walls even for small values of $\epsilon_{dd}$ (weakly interacting dipolar case, panels a,d and inset g) after the excitation spectrum of the uniform phase does not show a roton minimum. Due to the long range and anisotropic nature of the dipolar force, even in this case the density profile deeply differs from the results holding for a one-dimensional BEC interacting with a short range potential. In the latter case the density profile, near a hard wall located at $x = 0$, is fixed by the healing length $\xi = \sqrt{\hbar^2 / 2m g n}$ according to $n(x) = n_0 \tanh^2 (x/2\xi)$ where $n_0$ is the bulk density away from the edge of the box [11]. The concept of healing length is not easily applicable to the case of a dipolar gas, whose different behavior is due to the long-range nature of the force, the repulsive effect felt by the aligned dipoles, which tend to accumulate near the border, the presence, for large values of $\epsilon_{dd}$, of rotonic oscillations and, of course, the emergence of spontaneous density modulations characterizing the supersolid and the crystal phases. The emergence of the rotonic oscillations is reminiscent of a similar effect characterizing the density profile in the vicinity of a quantized vortex [51]. This effect, originally theoretically investigated for quantized vortices in superfluid helium, is a direct consequence of the presence of the roton in the excitation spectrum [52,53]. A similar behavior is observed along each edge of the polygonal box potentials shown in figures 3 and 4 of the main text, suggesting that such edge configurations host, between two vertices of the confining potential, localized excitations corresponding to those that naturally occurs in quasi one-dimensional configurations.

B. Roton energy for a quasi one-dimensional dipolar gas with periodic boundary conditions

In order to understand the (almost) uniform density phase appearing along the edges of the box configurations shown in figure [1] we have extended the results presented in [42,43] by studying the value of the roton excitation energy calculated for a quasi one-dimensional uniform dipolar gas in a transverse harmonic confinement, with periodic boundary conditions along the unconfined direction, as a function of the linear density $n = N/L$, where $n$ is the number of atoms and $L$ the length of the tube, and of $\epsilon_{dd}$. The results are shown in figure 5a. Notice that, for a fixed value of $\epsilon_{dd}$ above a critical threshold (here, $\approx 1.35$), increasing the density starting from small values (see the green dashed line), the system undergoes a transition from a superfluid to a supersolid phase, revealed by the instability of the roton minimum, to come back to the superfluid phase, characterized again by the occur-
rence of roton with a finite excitation energy, at larger values of the density.

FIG. S2. Roton energy of a quasi one-dimensional dipolar Bose gas with transverse harmonic confinement of frequencies $\omega_y = \omega_z = (2\pi)100\text{Hz}$, with periodic boundary conditions along the $x$ axis, as function of the linear density $n = N/L$, where $N$ is the number of atoms and $L$ the length of the simulation cell along $x$, and of $\epsilon_{dd}$. The blue dots correspond, from bottom to top, to the configurations of figure S1 panels d,e,f, while the white empty square corresponds to the the ring edge of the configuration shown in figure 4 panel e (circular transverse confinement). The dark area corresponds to configurations in which the roton mode, calculated starting from a uniform configuration, is unstable and where spontaneous density modulations of supersolid or crystal nature are formed. The green, horizontal dashed line is a guide to the eye showing that, for fixed $\epsilon_{dd}$, starting from a low-density superfluid, increasing the density results in a phase transition to a supersolid (and eventually to a droplet crystal), while at even higher densities the system turns superfluid again.