Supersolid behaviour of a dipolar Bose-Einstein condensate confined in a tube

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Motivated by a recent experiment [L.Chomaz et al., Nature Physics 14, 442 (2018)], we perform numerical simulations of a dipolar Bose-Einstein Condensate (BEC) in a tubular confinement at T=0 within Density Functional Theory, where the beyond-mean-field correction to the ground state energy is included in the Local Density Approximation. We study the excitation spectrum of the system by solving the corresponding Bogoliubov-de Gennes equations. The calculated spectrum shows a roton minimum, and the roton gap decreases by reducing the effective scattering length. As the roton gap disappears, the system spontaneously develops in its ground-state a periodic, linear structure formed by denser clusters of atomic dipoles immersed in a dilute superfluid background. This structure shows the hallmarks of a supersolid system, i.e. (i) a finite non-classical translational inertia along the tube axis and (ii) the appearance, besides the phonon mode, of the Nambu-Goldstone gapless mode corresponding to phase fluctuations, and related to the spontaneous breaking of the gauge symmetry. A further decrease in the scattering length eventually leads to the formation of a periodic linear array of self-bound droplets.

Dipolar Bose Einstein condensates (BECs) attracted great attentions in recent years, since the first experimental realizations of BECs with strongly magnetic atomic gases of $^{52}$Cr, $^{164}$Dy and $^{166}$Er [1–3]. This interest is motivated by the particular properties of such systems which are characterized by anisotropic and long-range dipole-dipole interactions in addition to the usual short-range contact interactions, resulting in a geometry dependent stability diagram [4] where the system (which is intrinsically unstable in 3D) becomes stable against collapse if the confinement along the polarization axis is much tighter that the in-plane confinement. The properties of dipolar BECs have been the subject of numerous experimental and theoretical studies, extensively reviewed in Ref.[5] and Ref.[6].

Recent experiments [7, 8] on the stability of a dipolar BEC of $^{164}$Dy trapped in a flat ”pancake” trap, under conditions where the gas is dominated by the dipolar interaction, showed the formation of droplets arranged in an ordered structure, their collapse being prevented by the tight confinement along the short axis. This effect is the equivalent of the Rosensweig instability of classical ferrofluids [9].

Remarkably, recent experiments [10] showed that self-bound droplets can be realized in a dipolar Bose gas depending upon the ratio between the strenghts of the long-range dipolar attraction and the short range contact repulsion. These droplets, whose densities are higher by about one order of magnitude than the density of the weakly interacting condensate, are stable even in free space, after the external trapping potential is removed.

The possibility of self-bound dipolar droplets has been explained theoretically in Ref.[11,12], where it has been shown that the binding arises from the interplay between the two-body dipolar interactions and the effects of quantum fluctuations. The latter can be embodied in a beyond-mean-field energy correction [13, 14], where a positive shift of the ground state energy with the Lee-Huang-Yang (LHY) form [15] counteracts the destabilizing effect of the dipole-dipole attraction. The crossover in a dipolar quantum fluid from a dilute BEC to self-bound macrodroplets was studied in Ref.[12], where further evidence was provided that quantum fluctuations indeed stabilize the ultracold gas far beyond the instability threshold imposed by mean-field interactions.

The properties of self-bound dipolar quantum droplets have been extensively studied from a computational point of view, both within a mean field theory approach that takes into account the LHY correction [11, 10], and with Quantum Monte Carlo simulations [17,19].

In Ref. [20] it has been shown that in a dipolar BEC of $^{166}$Er confined in a strongly prolate cygar-shaped trap ("tubular" trap), the reduction of the scattering length leads to the appearance of a roton mode, signalled by the presence, in the measured momentum distribution, of symmetric peaks at finite momenta. The excited states dispersion relation is thus characterized by a roton minimum, similarly to the case of $^4$He, the roton gap amplitude depending on the relative strengths of short-range and dipolar interactions. This suggests that when the roton gap becomes very small, a dipolar BEC confined in an axially elongated trap orthogonal to the polarization direction may develop a modulated density profile in its ground state. Based on this, it has been suggested [20] that this system may indeed show supersolid behavior.

The existence of a supersolid phase of matter was proposed long ago for $^4$He [21], but its experimental verification remained elusive [22]. The possibility of forming a solid structure simultaneously possessing crystalline and superfluid properties [23] is associated with an excitation spectrum of the liquid phase characterized by a roton minimum at finite k-vector [24], the liquid to supersolid...
transition being triggered by the vanishing of the roton gap. Supersolid phases have been recently predicted for confined condensed spinless bosons in 2-dimensions and 3-dimensions interacting via a broad class of soft core repulsive potentials. Supersolid behavior has been proposed for the stripe phase of a dipolar Bose gas moving in a plane when the polarization axis forms an angle with it. The only experimental evidence so far of supersolid behavior in cold gases has been reported recently in Ref. [28], where the authors realized an "infinitely stiff" supersolid of $^{87}\text{Rb}$ atoms with the density modulation artificially imposed by external optical lattices.

In this paper we study through numerical simulations based on T=0 Density Functional theory (DFT) within the Local Density approximation (LDA), the equilibrium structure and elementary excitations of a dipolar BEC confined in a tube whose axis is orthogonal to the polarization direction, and with periodic boundary conditions along the tube axis.

Within the DFT framework, the total energy of a dipolar BEC of atoms with mass $m$ and magnetic moment $\mu$ is:

$$E = \int \left[ \frac{\hbar^2}{2m} |\nabla \phi(r)|^2 + V_i(r) |\phi(r)|^2 + \frac{g}{2} |\phi(r)|^4 \right] dr + \frac{1}{2} \int V_{dd}(|r-r'|)|\phi(r)|^2|\phi(r')|^2 dr \, dr' + \frac{2}{5} \gamma(\epsilon_{dd}) \int |\phi(r)|^5 dr (1)$$

where $g = \frac{4\pi\alpha^2}{m}$, $a$ being the s-wave scattering length, $V_{dd}(r-r') = \frac{\mu_0 \mu^2}{4\pi}\frac{1-3\cos^2 \theta}{|\vec{r}-\vec{r}'|}$ is the dipole-dipole interaction between two identical magnetic dipoles aligned along the $z$ axis ($\theta$ being the angle between the vector $\vec{r}$ and the polarization direction $z$), and $\mu_0$ is the permeability of the vacuum. $V_i$ is the trapping potential. The last term is the beyond-mean-field (Lee-Huang-Yang, LHY) correction [13], where $\gamma(\epsilon_{dd}) = \frac{32}{\pi^3} g^2 a^2 F(\epsilon_{dd})$, $\epsilon_{dd} = \frac{\mu_0 \mu^2}{4\pi d^2}$ being the ratio between the strenghts of the dipole-dipole and contact interactions, and $F(\epsilon_{dd}) = \frac{1}{2} \int_0^\pi d\theta \sin \theta [1 + \epsilon_{dd}(3\cos^2 \theta - 1)]^\frac{3}{2}$. In the case of polar molecules the same expression for $V_{dd}$ applies, with $\mu_0 \mu^2$ replaced by $d^2/\epsilon_0$, where $d$ is the dipole electric moment of the molecule and $\epsilon_0$ is the vacuum permittivity. The number density of the dipole system is $n(r) = |\phi(r)|^2$.

The minimization of the above energy functional leads to the following Euler-Lagrange equation:

$$H_0 \phi(r) = \mu \phi(r) \tag{2}$$

with

$$H_0 = -\frac{\hbar^2}{2m} \nabla^2 + V_i(r) + g |\phi(r)|^2 + \int dr' |\phi(r')|^2 V_{dd}(r-r') + \gamma(\epsilon_{dd}) |\phi(r)|^4 \tag{3}$$

and $\mu$ is a Lagrange multiplier whose value is determined by the normalization condition $\int |\phi(r)|^2 dr = N$ (N being the total number of dipoles). In what follows $m$ is the mass of a $^{166}\text{Er}$ atom.

The same approach described by the previous equation has been used, e.g., in Ref. [14] and other papers addressing the effect of beyond-mean-field effects on the dipolar Bose gas. The predictions of the DFT-LHY approach described above has been tested in Ref. [17] against Quantum Monte Carlo simulations, showing that the DFT-LHY approach gives rather good results.

In the following we will assume a tubular confinement, i.e. the dipoles are radially confined by a harmonic potential $V_i(r) = \frac{1}{2} m (\omega_x^2 r^2 + \omega_z^2 z^2)$, in the $y-z$ plane ($z$ is the polarization direction and $y$ is the transvers direction). The harmonic frequencies are fixed to the values $\omega_x = \omega_z = 2\pi/(600)\text{Hz}$. This geometry closely matches the experimental set-up used in the recent experiments of Ref. [12, 20]. Along the third axis, $x$, the system is not confined, but subject to periodic boundary conditions (PBC), $\phi(x+L, y, z) = \phi(x, y, z)$, $L$ being the tube length.

Note that, due to the presence of PBC, the system is equivalent to a ring geometry (with a ring radius $R = L/2\pi$), if curvature effects can be neglected (i.e. when $R$ is much larger that the harmonic confinement length in the $y-z$ plane). This allows to test our prediction in actual experiments, where ring-shaped trapping potential can be easily realized.

Solution of equation (2) provides the ground-state configuration of the system. We solve this equation by propagating in imaginary time its time-dependent counterpart $i\hbar \frac{d\phi}{dt} = H_0 \phi$. In all the simulations we fix the value of the linear density $n_0 = N/L$ and vary the value of the ratio, $\epsilon_{dd}$, between the dipolar and contact interaction strengths. The total number of atoms is fixed to $N = 4 \times 10^4$. To compute the spatial derivatives appearing in the equation (2), we used an accurate 13-point finite-difference formula. The convolution integral in the potential energy term of Eq. (2) is efficiently evaluated in reciprocal space by using Fast Fourier transforms, recalling that the Fourier transform of the dipolar interaction is $\tilde{V}_k = (\mu_0 \mu/3)(3\cos^2 \alpha - 1)$ where $\alpha$ is the angle between $\mathbf{k}$ and the $z$-axis.

In order to study the elementary excitations, we expand the wave function in the Bogoliubov-de Gennes (BdG) form $\Psi(r,t) = e^{-i\mathbf{k} \cdot \mathbf{r}} |\phi(r) + u(r)e^{-i\omega t} - v^*(r)e^{i\omega t}|$, and insert this expansion in Eq. (2). Keeping only terms linear in the amplitudes $u$ and $v$, one gets the BdG equa-
tions for the amplitudes $u$ and $v$ and the excitation energies $\epsilon$, that can be cast in a matrix form as:

\[
\begin{pmatrix}
H_0 - \mu + \hat{X} & -\hat{X}^\dagger \\
\hat{X} & -H_0 + \mu + \hat{X}^\dagger
\end{pmatrix}
\begin{pmatrix}
u \\
v
\end{pmatrix}
= \epsilon
\begin{pmatrix}
u \\
v
\end{pmatrix}
\] (4)

where $H_0$ is given in Eq. (3) and the operator $\hat{X}$ is defined by its action on the function $f$ as

\[
\hat{X}f(r) = \phi(r) \int dr' [V_{dd}(r - r') + g\delta(r - r')]|\phi^*(r')f(r') + \frac{3}{2} \gamma(\epsilon_{dd})|\phi(r)|^3 f(r)
\]

(5)

Because of our use of Fourier transforms, which imply that PBC must be imposed in our calculations, we can expand the wavefunction $\phi$ and the complex functions $u, v$ in the Bloch form appropriate to a periodic system. In this way, the equations (4) can be solved in reciprocal space allowing to find $\epsilon_k$ in the right-hand side of Eq. (4) (see Ref. [26] for details about the numerical methods used to solve Eq. (4)).

We first solve the BdG equations to compute the excitation spectrum for a dipole system characterized by a uniform density along the tube axis (x-axis). The energies $\epsilon_k$ of the mode along the $k_x$ direction are shown in Fig. 1 for the choice $n_0 = 0.2a_0^{-1}$, where $a_0$ is the Bohr radius, for different values of $\epsilon_{dd}$. Notice that, as $\epsilon_{dd}$ is increased (i.e. the scattering length $a$ is decreased), a roton minimum develops in the dispersion relation, eventually vanishing at $\epsilon_{dd} = 1.45$.

This signals a possible density modulation instability that might break the uniform symmetry along the tube axis. In order to verify this, we calculated the ground-state density profile by solving the Eq. (2) for different values of $\epsilon_{dd}$. In Fig. 1 we show the ground state density for two different values of $\epsilon_{dd}$. As the typical imaging techniques in experiments allows to measure the density of the BEC integrated along the viewing direction, we plot in Fig. 1 the density $n_z(x, y) = \int n(x, y, z)dz$ integrated along the $z$-axis. One can see that the ground state density remains uniform along the tube for finite values of the roton gap, while it becomes periodicaly modulated as the roton gap vanishes. The resulting structure in the latter case is shown in the lower panel of Fig. 1. The periodicity of the density profile is $\lambda = \frac{2\pi}{k^c_x}$, where $k^c_x$ is the critical value of the momentum at which the roton gap vanishes.

The periodic structure corresponding to $\epsilon_{dd} = 1.45$ appears to be made of regularly arranged, dense clusters of dipoles immersed in a background of very dilute condensate (the background density being one order of magnitude smaller than the cluster density at $\epsilon_{dd} = 1.45$, and about 100 times smaller at $\epsilon_{dd} = 1.52$). This suggests that the systems, for $\epsilon_{dd} > 1.45$ may display a supersolid character. In order to verify this hypothesis, we have looked for the characteristic hallmarks of supersolid behavior of the modulated structures, i.e. [29] (i) a finite non-classical translational inertia and (ii) the appearance, besides the phonon mode, of a gapless ”super-fluid band” resulting from the spontaneous breaking of global gauge symmetry.

![FIG. 1: Upper panel: dispersion relation of excitations propagating along the axis of the tube (of length $L$) in the homogeneous system. Energies are in atomic units. Lower panel: integrated density $n_z(x, y)$ below and at the critical value of $\epsilon_{dd}$ where the roton gap vanishes. The total number of atoms is $N = 4 \times 10^4$.](image-url)
First, we check the presence of Non-Classical Translational Inertia (NCTI). This is done by solving for stationary states the real-time version of the EL equation \( \frac{\partial}{\partial t} \phi(r) = (H_0 + i\hbar v_x \frac{\partial}{\partial x})\phi(r) \) in the comoving reference frame with uniform velocity \( v_x \), i.e.

\[
i\hbar \frac{\partial}{\partial t} \phi(r) = (H_0 + i\hbar v_x \frac{\partial}{\partial x})\phi(r)
\]

Following Ref. [29], we define the superfluid fraction \( f_s \), as the fraction of particles that remains at rest in the comoving frame:

\[
f_s = 1 - \frac{\langle P_x \rangle}{Nmv_x}
\]

where \( \langle P_x \rangle = -i\hbar \int \phi^* \frac{\partial \phi}{\partial x} \) is the expectation value of the momentum and \( Nmv_x \) is the total momentum of the system if all the particles were moving.

We can see from figure 2 that, when a modulation in the density profile appears, the superfluid fraction becomes smaller than one, and it decreases as \( \epsilon_{dd} \) is increased.

Another evidence of supersolid behavior is associated with the presence in the excitation spectrum of the periodically modulated structure shown in figure 1, of an extra gapless mode besides the usual phonon modes. The excitation spectrum can be calculated by solving the corresponding BdG equations for modes propagating along the axis of the tube. The result is shown in figure 2, for the values \( \epsilon_{dd} = 1.45 \) and \( n_0 = 0.2 a_0^{-1} \), from which one can see the appearance of two Goldstone (gapless) modes associated with symmetry breaking. The harder mode is associated to the density response of the system, and it corresponds to the usual “phonon” branch. The softer mode is associated instead to the phase response of the system, and it signals the partial superfluid character of the supersolid (Nambu-Goldstone mode). (The correct mode assignment was made by looking at the calculated local density and phase fluctuations [26, 30], \( \Delta \rho(r) = \sum_{n,k} |u_{n,k} - v_{n,k}|^2 \) and \( \Delta \theta(r) = \sum_{n,k} |u_{n,k} + v_{n,k}|^2 \), respectively).

From Fig. 2 (upper panel) it appears that as \( \epsilon_{dd} \) increases, the superfluid fraction tends to zero. When this happens, the atomic clusters shown in the lowest panel of Fig. 1 begin to merge, forming denser isolated droplets, while the calculated energy per particle becomes negative, as shown in Fig. 3. This happens at \( \epsilon_{dd} \sim 1.72 \).

Above this value, the ground state of the system takes the form of an (ordered) one-dimensional lattice of self-bound quantum droplets (each containing \( N = 10^4 \) atoms), while the supersolid behaviour is completely suppressed, as shown by the disappearance of the Nambu-Goldstone mode from the calculated excitation spectrum.

The inverse compressibility of the system \( \kappa^{-1} = -V \frac{\partial^2 E}{\partial V^2} \) can be easily computed by static calculations with a fixed number of particle \( N \), where the length of the tube is varied while the transverse confinement remains unchanged. In figure 3, we show \( \kappa^{-1} \) as a function of \( \epsilon_{dd} \). One can see that, whereas the supersolid phase turns out to be extremely compressible, as the supersolid behaviour is suppressed the inverse compressibility quickly rises, i.e. the compressibility of the system decreases. This is due to the repulsive interaction between the self-bound droplets which behave as giant aligned dipoles repelling each other.

In conclusions we have shown, by means of numerical simulations based on the DFT-LHY approach, that in a dipolar BEC confined in a tube at \( T = 0 \) the softening of the roton mode, caused by a decrease in the scattering length, leads to the formation of a modulated structure in the ground state of the system, in which denser clusters of dipoles are immersed in a very dilute superfluid background. This system shows the hallmarks of supersolid behaviour, i.e. a finite, non-classical translational inertia, and an additional Goldstone "superfluid" mode in the excitation spectrum. The supersolid behaviour is suppressed when the system, by further decreasing the
scattering length, enters in a regime in which the dipole clusters turn into an ordered array of self-bound quantum droplets.

The phase coherence of the supersolid phase described here could be experimentally detected in a dipolar condensate confined in a ring trap where, after having tuned the scattering length across the threshold value required for the supersolid formation, the trapping potential is switched off, allowing the atomic wavefunction to expand freely. By doing subsequent absorption imaging one could detect the presence of interference maxima associated with phase coherence[28].

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