Static and Dynamic Study of Bose-Einstein Condensates

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Abstract: The aim of the project is to study the formalism behind Bose-Einstein condensates. Using the imaginary time method, we obtain the ground state of the condensate solving the Gross-Pitaevskii equation with an ansatz wave function. Then, we study the two analytical limit cases: the Thomas-Fermi approximation and the non-interacting limit. After that, we perturb the condensate with the monopolar excitation operator and we observe the oscillations produced on the expectation value of $\langle r^2 \rangle$. We obtain the frequency of the oscillations of the condensate with a Fourier transform analysis. Finally, we expand our study considering a contribution beyond the mean-field theory in order to study the emergence of self-bound droplets. We compute the ground state for this system, following the same procedures as for the condensate.

I. INTRODUCTION

At very low temperatures, matter can behave in two very different ways: as fermions or as bosons. Fermions are particles with half-integer spin and interfere destructively between them, while bosons are particles with integer spin which interfere constructively. Although most of the fundamental matter are fermions (protons, electrons, neutrons), by putting together an even number of fermions so their spins are coupled to make a total, integer spin, one ends up having a system that behaves as a boson. The Pauli exclusion principle is the crucial difference between the two types of particles: two fermions cannot occupy the same quantum state, but we can have any number of bosons in the same state. This last property, along with the indistinguishability of the particles, make bosons interesting to study, specially if we cool them to very low temperatures.

If we cool down a bosonic dilute gas close to 0 K, almost all the atoms of the system occupy the lowest single-particle energy state. As a knock-on effect, they lose their individual properties and the whole system starts to behave as a single collective quantum wave that follows the Bose-Einstein statistics. Quantum effects become macroscopic. This behaviour was predicted almost 100 years ago by Satyendra Nath Bose and Albert Einstein. Since then, Bose-Einstein condensation has been one of the most studied phenomenon in quantum sciences. Nevertheless, it was not until 1995 that a research group at the Joint Institute for Laboratory Astrophysics (JILA) produced the very first quantum condensate. It was composed of 2000 ^{87}Rb atoms and cooled down to temperatures of nanokelvin [3].

After some years of investigation, in 2015 D. S. Petrov demonstrated that self-bound droplets, without any external confinement, could be produced in bosonic binary mixtures by extending the Gross-Pitaevskii formalism to account for quantum fluctuations [7]. Then, three years later, in 2018, the first quantum droplets were observed as heteronuclear mixtures of ^{41}K and ^{87}Rb. Even so, this liquid-like behaviour was first noticed in dipolar condensates and in homonuclear mixtures of ^{39}K [6]. In order to obtain these droplets, we need to have competing mean-field interactions so they can compensate with the quantum fluctuations of the system. We can achieve this with heteronuclear mixtures, where we have contact interactions between atoms of the same type and between atoms of different component. In addition, we can tune these interactions in order to achieve larger lifetimes so droplets can be observed in an easier way.

This project aims at studying the theoretical mean-field description of Bose-Einstein condensates. First, we will numerically obtain the ground state and check it with the analytical limits. Then, we will perturbe it with a monopolar excitation. Finally, we will extend the mean-field formalism to account for quantum fluctuations and obtain self-bound droplets. We will study in what they differ from ordinary condensates and we will compute the ground state for the self-bound droplet.

II. BOSE-EINSTEIN CONDENSATES

We consider N identical bosons at $T = 0$ K and assume that the system is very dilute and weakly-interacting. In such a low density system, the interacting potential can be described as an effective contact potential which only depends on the s-wave scattering length of the particles. This is, therefore, a mean-field approximation, as we can assume every particle feels the same effective potential. Furthermore, if the interactions between atoms are attractive, then our system will collapse in any circumstance. If it is repulsive, then the system expands so we need a confinement method in order to have a bounded system. This means that in order to have a Bose-Einstein condensate (BEC), an external, confining potential is needed.

At a very low temperature, thermal fluctuations can

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be neglected, so we can consider that almost all atoms are condensed, and due to the diluteness and weak interactions, quantum fluctuations are also negligible. Under this conditions, the system is within the mean-field regime and can be described by the time-dependent Gross-Pitaevskii equation [8], which is enunciated as

$$\left[-\frac{\hbar^2\nabla^2}{2m} + V_{\text{ext}}(\vec{r}) + gN|\Psi(\vec{r},t)|^2\right]\Psi(\vec{r},t) = i\hbar\frac{\partial}{\partial t}\Psi(\vec{r},t), \tag{1}$$

where the first term refers to the kinetic energy and the second one is the external, confining potential mentioned before. Contact interactions are characterized by the coupling constant $g = 4\pi\hbar^2 a_s/m$, which depends on the s-wave scattering length a_s, and N is the number of particles. As said before, we need interactions to be repulsive, so g will be positive. It is important to mention that Eq. (1) provides a good description of BECs as long as the conditions described before regarding thermal and quantum fluctuations are maintained. We also assume that densities are still low enough to avoid losses due to three-body interactions.

Aiming to obtain an expression for the ground state of the condensate, since it is a stationary state, we can split our wave function in two parts: the first one contains the spatial dependence and the second one the time dependence, as

$$\Psi(\vec{r},t) = \varphi(\vec{r})\,\exp\left(-i\mu t/\hbar\right), \tag{2}$$

where μ is the chemical potential. Inserting this wave function into Eq. (1) we obtain the time-independent Gross Pitaevskii equation (GPE),

$$\left[-\frac{\hbar^2\nabla^2}{2m} + V_{\text{ext}}(\vec{r}) + gN|\varphi(\vec{r})|^2\right]\varphi(\vec{r}) = \mu\,\varphi(\vec{r}). \tag{3}$$

III. BEC WITH HARMONIC CONFINEMENT

We consider a BEC confined in an isotropic harmonic trap of frequency ω, $V_{\text{ext}}(r) = m\omega^2 r^2/2$. To facilitate calculations, we write these equations in harmonic oscillator units, with $a_{\text{ho}} = \sqrt{\hbar/(m\omega)}$ as the length unit, $\hbar\omega$ as the energy unit and ω^{-1} as the time unit. Then we write dimensionless positions, wave functions, energies and chemical potentials as $\overline{r} = r/a_{\text{ho}}$, $\overline{\varphi}(\overline{r}) = a_{\text{ho}}^{3/2}\varphi(\overline{r})$, $\overline{E} = E/(\hbar\omega)$ and $\overline{\mu} = \mu/(\hbar\omega)$. We rewrite Eq. (1) as

$$\left[-\frac{\nabla^2}{2} + \frac{1}{2}\overline{r}^2 + gN|\overline{\varphi}(\overline{r},t)|^2\right]\overline{\varphi}(\overline{r},t) = i\frac{\partial}{\partial t}\overline{\varphi}(\overline{r},t), \tag{4}$$

where $g = 4\pi\overline{a}$ and $\overline{a} = a_s/a_{\text{ho}}$. Eq. (3) becomes

$$\left[-\frac{\nabla^2}{2} + \frac{1}{2}\overline{r}^2 + gN|\overline{\varphi}(\overline{r})|^2\right]\overline{\varphi}(\overline{r}) = \overline{\mu}\,\overline{\varphi}(\overline{r}). \tag{5}$$

A. Ground State

In this section we will numerically obtain the ground state of the system by means of the imaginary time method. We wrote a Fortran program that included this method. It sets the time of the differential equation as an imaginary time $\tau = -i\,t$, so the equation becomes a diffusion equation. For long enough times, it is guaranteed that the method converges to the ground state of the system starting from any initial wave function.

First, we solve the GPE for different number of particles using the following initial wave function:

$$\phi_0(\mathrm{r}) = \alpha\,\mathrm{r}\,\mathrm{e}^{-\beta\mathrm{r}^2}, \tag{6}$$

where α and β are both constants. We solve Eq. (5) with the imaginary time method, where $\overline{\mu}$ is calculated as

$$\overline{\mu} = \frac{1}{N}\int d\vec{r}\,\phi^*(\overline{r})\,\hat{\mathcal{H}}\,\phi(\overline{r}), \tag{7}$$

with $\hat{\mathcal{H}}$ defined as

$$\hat{\mathcal{H}} = -\frac{\nabla^2}{2} + \frac{1}{2}\overline{r}^2 + gN|\overline{\phi}(\overline{r})|^2. \tag{8}$$

The results for the ground state are shown in Fig. 1 for different number of atoms.

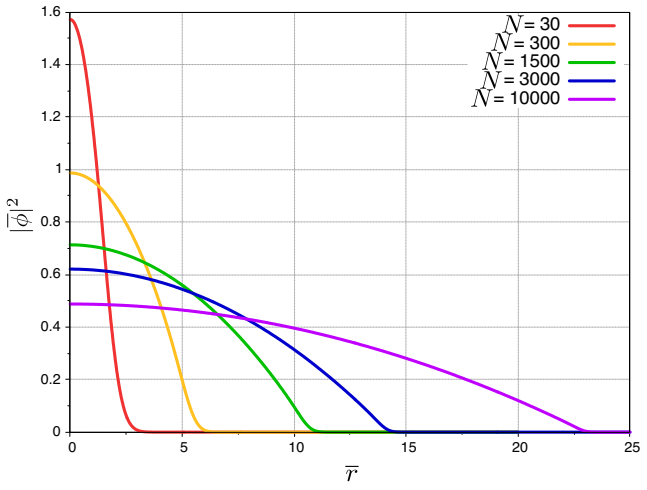

FIG. 1: Density profile of the Bose-Einstein condensate ground state in dimensionless units and for different number of atoms.

It is interesting to see that we recover the two analytical limits for large and small number of particles [4].

For large N, when $\overline{a}\,N \gg 1$, the Thomas-Fermi (TF) limit is achieved. The kinetic energy can be neglected in front of the interaction term, and an analytical solution of the GPE can be obtained. This can happen in two situations: if the kinetic term is very small and/or if the interaction term is very big, which is the case here. As this last one increases linearly with N, for big N the

kinetic part of the hamiltonian is negligible. Graphically, the approximation can be seen as the turning point near zero of the density disappears, so the density profile is almost an inverted parabola. Given our parameters, for $N = 10000$ the TF approximation is valid.

For small N the non-interacting limit is achieved, when the interaction term can be neglected in front of the kinetic energy. In this limit, the ground state is a gaussian. Note that the interaction term is the only one that depends on N, so if we reduce enough the number of particles, this term is negligible with regard to the kinetic and the external potential ones. In the system we are studying, for $N = 30$ the non-interacting limit is achieved.

B. Dynamic Evolution: monopolar excitation

Now we will study the dynamic evolution of the condensate. To evaluate the response of the system to a small perturbation, a superior order integration method will be used to solve the time-dependent differential equation (4). In this case, we use the 4th order Runge-Kutta method to solve it. Here, the Fortran program we need to write is more simple than the imaginary time one but it is harder in terms of running time. For each iteration, we solve the equation in every position of the grid in parallel.

Before studying the dynamical evolution, we have tested the ground state solution obtained by solving Eq. (5). For this purpose, we introduce the numerical wave function obtained before in the time-dependent GPE (4). As expected, the wave function does not change at all and preserves its normalization, that is, no particles are being lost or gained in the process. Gaining particles does not have any physical sense but it can happen with numerical methods. In fact, the number of particles oscillates around the correct normalization value.

Now we are going to introduce the perturbation to the condensate to study its dynamical response. In order to study its time evolution, we will proceed following two steps. First of all, we calculate a perturbed ground state with the static method explained previously. After that, we switch off the perturbation and we let the condensate evolve. We can introduce the perturbation in two different ways: we can change the harmonic oscillator frequency, which means changing the parameters of the harmonic oscillator units, as we cannot find ω explicitly in the reduced equations, or we can introduce to our hamiltonian the monopolar excitation operator, λr^2, which excites the so called "breathing mode". We tried both perturbing methods but the presented results were calculated with the monopolar excitation operator. In fact, both methods are equivalent, as we are changing the multiplying factor of r^2. We set $\lambda = 10^{-6}$. It is a small perturbation but it is enough to see how the condensate evolves and oscillates.

At this point, we introduce the perturbed wave function in the dynamical code to study the real time evolution. Since we are exciting the monopolar (breathing) mode, in order to study the dynamical evolution of the BEC we compute $\langle r^2(t)\rangle$. Afterwards we will use Fourier analysis to obtain the frequencies of oscillation of the condensate. Results for a condensate of $N = 20000$ atoms are shown in Figs. 2 and 3.

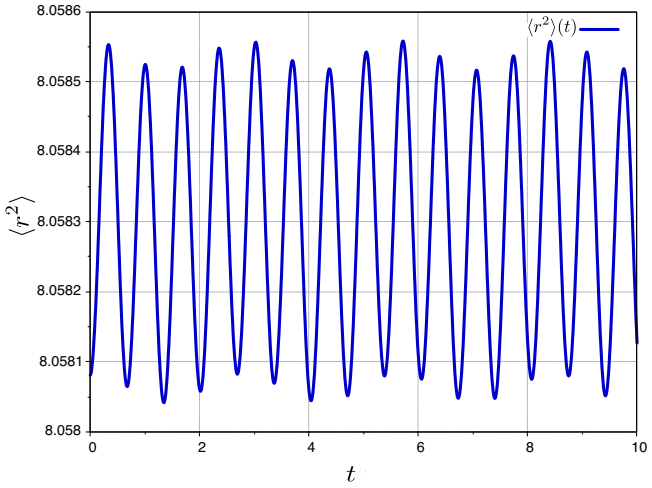

FIG. 2: Expectation value of r^2 as a function of time for the oscillations of the perturbed condensate in dimensionless units. Several periods are presented.

Figure 2 shows that the condensate oscillates following two differentiated periodical wave oscillations: on the one hand, the amplitude of the wave oscillates periodically with time, describing a main sinusoidal shape. On the other hand, a smaller frequency modulates the main oscillation also in a sinusoidal shape. The frequency of the main wave is bigger than the frequency of the modulation wave. This shape may be approximated as a sum of two oscillations described as

$$f(t) = A\,\cos(\overline{\omega}_1\,t) + B\,\cos(\overline{\omega}_2\,t), \tag{9}$$

where $\overline{\omega}_1$ corresponds to the main frequency and $\overline{\omega}_2$ to the modulation one. In addition, $A/B \approx 10$ and $\overline{\omega}_1/\overline{\omega}_2 \approx 4.5$. This result has been obtained empirically.

Figure 3 shows the results of the Fourier spectra analysis performed to our condensate from Fig. 2 in dimensionless units. It is shown that as a whole, it oscillates at a frequency around $\omega_1 = 9.43$. Then, we find another peak around $\omega_5 = 2.09$, with a lower strength compared to the first one. If we substitute ω_1 and ω_5 in Eq. (9), we can see they verify $\omega_1/\omega_5 \approx 4.5$. It is worth mentioning that frequency $\omega = 0$ has been excluded from the spectra as it is considered noise associated with the finite dimensions of the system.

Once we have analysed the numerical results, now we can compare them with the analytical predictions. In the TF limit, it has been shown in Refs. [4, 8] that the frequency for the monopolar mode admits an analytical expression: $\omega_{\mathrm{M}} = \sqrt{5}$ (in units of the trap frequency). If we compare this value with our results, it is clear that ω_5

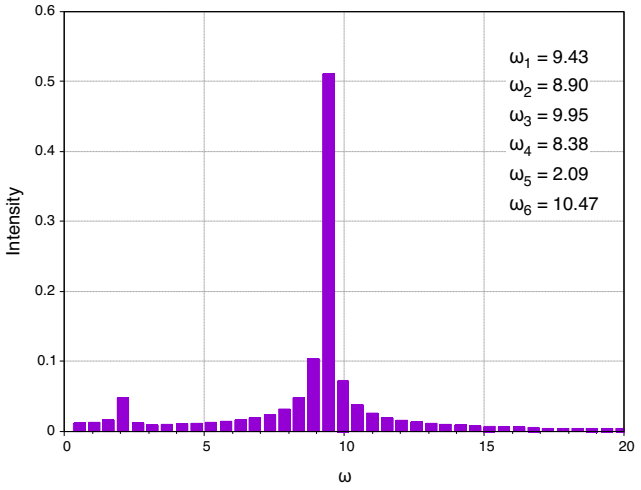

FIG. 3: Frequency spectrum of the condensate oscillations in dimensionless units. The top right label presents the six frequencies obtained with decreasing strength.

corresponds to the monopolar mode, as its value is very close to ω_{M}. The large-frequency oscillations that we observe at frequency ω_1 may be a result of the perturbation not being small enough. As a result, besides the oscillation related to the monopolar excitation we observe a second oscillation because the perturbation might be exciting other modes. The larger strength for ω_1 that we see on the frequency spectrum is related to the number of periods that we consider, which is much larger for the large-frequency oscillations.

IV. SELF-BOUND DROPLETS

Now that we have studied how a Bose-Einstein condensate behaves under a monopolar perturbation, we consider beyond mean-field effects to investigate self-bound quantum droplets.

As mentioned in the introduction, in order to achieve the droplet state, we need to expand our study with two considerations. First, our system will need to be a mixture of two different species in order to have competing mean-field interactions within the condensate: we will have inter-species and intra-species interactions. This means that we now have different interaction constants g that will be described later in this section. Then, with the purpose of getting our self-bound droplet, we need to consider a beyond mean-field contribution so we can take into account quantum fluctuations. These quantum fluctuations can stabilize the system against the collapse predicted by the mean-field framework. This contribution is the Lee-Huang-Yang (LHY) correction [5].

For very dilute and weakly-interacting systems, quantum fluctuations are usually neglected. However, there are systems where the mean-field energy can be very low and become of the order of magnitude of quantum fluctuations. This happens when there are competing mean-field interactions within the condensate and the density is large enough so quantum fluctuations are significant. In this case, then, the balance between the attractive mean-field interactions and the repulsive quantum fluctuations leads to equilibrium at a given density where the mean-field theory would predict collapse.

If we consider our ^{41}K-^{87}Rb mixture has an attractive interaction potential, in the absence of an harmonic trap the system should collapse. If we contemplate quantum fluctuations and we add this repulsive LHY correction to our maths, then the condensate can stabilize and sustain itself. This attractive-repulsive compensation that we achieve permits us to set the external potential equal to zero and still get a self-bound system. This system described is named a self-bound quantum droplet.

Mathematically, the following formalism was presented by D.S. Petrov in [7]. Altough this binary system is described by two coupled GPEs, for the ground state and the lowest energy states of the system we can effectively model it as a one component system, neglecting the relative motion between species. If we write the GPE in dimensionless form and we add the LHY correction $5/2|\phi|^3 - \tilde{\mu}$ we get

$$\left[-\frac{\nabla_{\tilde{r}}^2}{2} - 3|\phi(\tilde{r},\tilde{t})|^2 + \frac{5}{2}|\phi(\tilde{r},\tilde{t})|^3 - \tilde{\mu}\right]\phi(\tilde{r},\tilde{t}) = i\frac{\partial}{\partial\tilde{t}}\phi(\tilde{r},\tilde{t}) \tag{10}$$

Where $\tilde{\mu}$ is the dimensionless chemical potential and $\tilde{r}$, $\tilde{t}$ are the rescaled position and time coordinates, $\tilde{r} = r/\xi$ and $\tilde{t} = t/\tau$, being ξ and τ:

$$\xi = \sqrt{\frac{3}{2}\frac{\sqrt{g_{22}}/m_1 + \sqrt{g_{11}}/m_2}{|\delta g|\sqrt{g_{11}}n_1^{(0)}}}, \quad \tau = \frac{3}{2}\frac{\sqrt{g_{22}} + \sqrt{g_{11}}}{|\delta g|\sqrt{g_{11}}n_1^{(0)}}, \tag{11}$$

where m_1 and m_2 are the masses of the two components, $n_1^{(0)}$ is the density of the first component, g_{ij} represents both the intra-species ($i = j$) and the inter-species ($i \neq j$) contact interactions, and $|\delta g| = g_{12} + \sqrt{g_{11}g_{22}}$. Solving Eq. (10) we obtain the ground state wave function of the self-bound droplet.

A. Ground state

All the computation used to obtain the ground state for the condensate can be recycled in this section. We only need to change the non linear potential terms from the GPE for the one that appears in Eq. (10), and set the external potential to zero. In addition, we put $\partial_{\tilde{t}}\phi(\tilde{r},\tilde{t}) = 0$ in Eq. (10) so we get the time-independent extended GPE, the one we need to solve, as it follows

$$\left[-\frac{\nabla_{\tilde{r}}^2}{2} - 3|\phi(\tilde{r})|^2 + \frac{5}{2}|\phi(\tilde{r})|^3\right]\phi(\tilde{r}) = \tilde{\mu}\phi(\tilde{r}). \tag{12}$$

We follow the same steps as we did to find the ground state of the condensate: we solve our equation iteratively

and we calculate $\tilde{\mu}$ as in Eq. (7) to evaluate it. After several iterations we obtain what is shown in Fig. 4 for different number of particles.

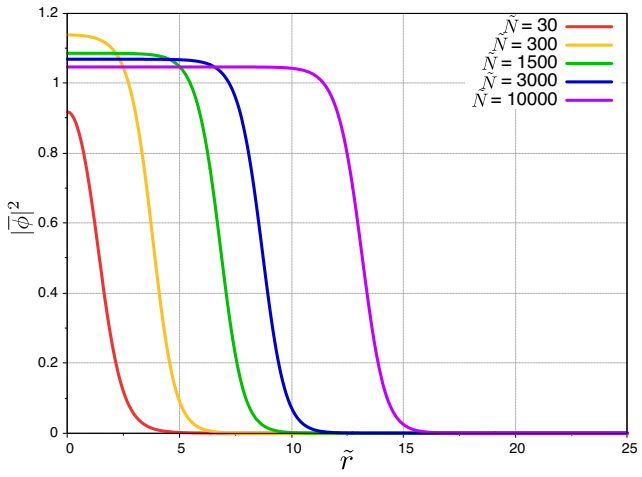

FIG. 4: Density profile of the self-bound droplet ground state in dimensionless units and for systems with different number of particles.

We can clearly see that by increasing the number of particles of the droplet, the bulk grows until it reaches saturation. We can now compare Fig. 1 with Fig. 4. For a small number of particles, the density profiles of both systems are almost the same, for droplets we also recover the gaussian distribution. It is worth mentioning that for $\tilde{N} = 18.65$ the droplet becomes unstable and can no longer contain itself as the kinetic term of the total energy is big enough compared to the rest of the terms [7]. For a large number of particles, both behaviours differ from each other. While for the condensate we recover the inverted parabola of the TF approximation, the droplet increases its bulk and saturates due to being self-bound.

V. SUMMARY AND CONCLUSIONS

In this project, we have studied the theoretical mean-field description of Bose-Einstein condensates in both the static and the dynamic regimes. Then, we have taken into account a beyond mean-field correction (known as the Lee-Huang-Yang correction) in order to obtain self-bound droplets.

First, we studied the mathematical formalism of Bose-Einstein condensates: how it can be explained by means of the Gross-Pitaevskii equation and why we need every term of the equation. Then, using the imaginary time method, we computed the ground state of the BEC and we checked its analytical limits: for large number of particles we recovered the TF approximation while for small number of particles we recovered the non-interacting limit, where the density profile is a gaussian. Once we had the ground state of the condensate, we introduced a perturbation with the aim of exciting the monopolar mode (also known as the breathing mode). We evolved the numerical wave function obtained from the static study with the perturbation and then we analysed the frequency oscillations using a Fourier transform analysis.

With all the condensate formalism developed, we have included quantum fluctuations in our GPE formalism in order to obtain self-bound droplets. We have studied under what circumstances they can be produced and stabilized: taking into account the Lee-Huang-Yang correction for quantum fluctuations. We have seen that we need competing mean-field interactions so the mean-field contribution is small and comparable to the quantum fluctuations. It is due to this balance between mean-field interactions and quantum fluctuations that droplets are self-bound systems. Finally, via this extended GPE (including the LHY correction) we obtained mumerically the ground state of a droplet the same way it was done for the condensate, and we discussed the differences between the density profiles of BECs and droplets for different number of atoms.

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[1] F. Böttcher *et al.*, *New states of matter with fine-tuned interactions: quantum droplets and dipolar supersolids* (Rep. Prog. Phys. 84 012403 (2021))
[2] Eric A. Cornell, *Very Cold Indeed: The Nanokelvin Physics of Bose-Einstein Condensation* (J. Res. Natl. Inst. Stand. Technol. 101, 419 (1996))
[3] Eric A. Cornell; Carl E. Wieman, *The Bose-Einstein Condensate* (Sci. Am. (1998))
[4] F. Dalfovo *et al.*, *Theory of Bose-Einstein condensation in trapped gases*, (Rev. Mod. Phys., Vol. 71, No. 3 (1999))
[5] I. Ferrier-Barbut, *Ultradilute Quantum Droplets* (Physics Today 72, 4, 46 (2019))
[6] C. Fort; M. Modugno, *Self-Evaporation Dynamics of Quantum Droplets in a* ^{41}K-^{87}Rb *Mixture* (Appl. Sci. 11, 866 (2021))
[7] D. S. Petrov, *Quantum Mechanical Stabilization of a Collapsing Bose-Bose Mixture* (Phys. Rev. Lett. 115, 155302 (2015)).
[8] L. Pitaevskii; S. Stringari, *Bose-Einstein condensation and superfluidity* (Oxford University Press, Vol. 164 (2016))
[9] S. T. Thornton, J. B. Marion, *Classical Dynamics of Particles and Systems* (2004)