Weakly interacting and confined bosons at low density

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1   Introduction

Given N identical bosons trapped in a harmonic potential at temperatures near 0K with a contact interaction between particles, the system can be described in a very good approximation by the Gross-Pitaevskii Equation. Assuming that all particles occupy the same monoparticular state, the equation describes how the best single-particle state to describe the N particles behaves. Taking $N >> 1$, the contact interaction as $V(|\vec{r_1} - \vec{r_2}|) = \frac{4\pi\hbar^2 a_s}{m}\delta^{(3)}(\vec{r_1} - \vec{r_2})$ and assuming spherical symmetry, the radial part of the equation, in harmonic oscillator units, reads

$$\bar{\mu}\overline{\varphi}(r_1) = \left[-\frac{1}{2}\frac{d^2}{dr^2} + \frac{1}{2}r_1^2 + \bar{a}_s N|\overline{\varphi}(r_1)|^2 \right]\overline{\varphi}(r_1). \tag{1}$$

The objective of this assignment is, given 5 different experiments of Bose Einstein Condensates of ^{87}Rb, as shown in table 1, find the $\Psi(\vec{r_1})$ ground state and calculate the chemical potential and energy of the system, finding the different contributions of each term of the GP equation to it, the density profile, and finally check if Virial's Theorem is fulfilled. We will also do the analysis using the Thomas-Fermi approximation, and we will compare the different results we obtain.

Since the equation is non linear, for each experiment $\overline{\Psi}(\vec{r_1})$ will need to be calculated iteratively. To get to the solution of the equation then, an initial gaussian-like wave function

$$\phi(r_1) = 2\sqrt{\frac{\alpha^3}{\sqrt{\pi}}}e^{-\frac{\alpha^2 r_1^2}{2}} \tag{2}$$

in a discretized space is given in order to evolve it numerically until it converges to the actual ground state of system. To do so, the evolution is performed in small steps in imaginary time $\tau = it$ and expanding the evolution operator up to second order:

$$e^{-H\tau} = 1 - H\tau + \frac{1}{2}H^2\tau^2 + O(\tau^3), \tag{3}$$

Where H is the operator that appears in the GP equation that has μ as its eigenvalue and that collapses the amplitudes of its eigenfunctions based on the value μ. If applied iteratively then, and by renormalizing at each step ($e^{-H\tau}$ is a diffusion operator that does not conserve normalization), the state ends up evolving into the ground state of the system, which has the minimal chemical potential, where the properties of the condensate can be studied.

In terms of implementation, the simulation has been done using Python. The Jupyter Notebook containing all the documented code used as well as some extra visualizations/illustrations, can be found along this document in the submitted folder or in the GitHub repository of the project.

2   Non interacting case

Before tackling the interacting case, we first solve the system without any interaction between the particles for experiment 1 but setting the scattering length to 0.This case has an analytical gaussian solution which in harmonic oscillator units reads

$$\overline{\varphi}(r_1) = 2\left(\frac{1}{\pi}\right)^{1/4}e^{\frac{-r_1^2}{2}}. \tag{4}$$

Experiment	A0	N1	STEP	AA	TIME	ALPHA	ITER
1	0.00433	700	0.015	1000000	0.00005	0.3	70000
2	0.00433	400	0.015	10000	0.00010	0.8	40000
3	0.00433	600	0.015	100000	0.00010	0.4	50000
4	0.00433	400	0.020	1000	0.00010	0.5	50000
5	0.00433	300	0.020	100	0.00010	0.5	50000

Table 1: Table of the data for the different experiments studied in this work. The different variables have the following meaning: A0: Values of the scattering length of the interaction between the rubidium atoms. N1: Number of grid steps in the discretized coordinate space. STEP: Step size of the coordinate grid. AA: Number of atoms, equivalent to N. TIME: Time step for the evolution. ALPHA: Parameter that adjusts the width of the initial Gaussian wave-function. ITER: Number of time-steps of evolution performed.
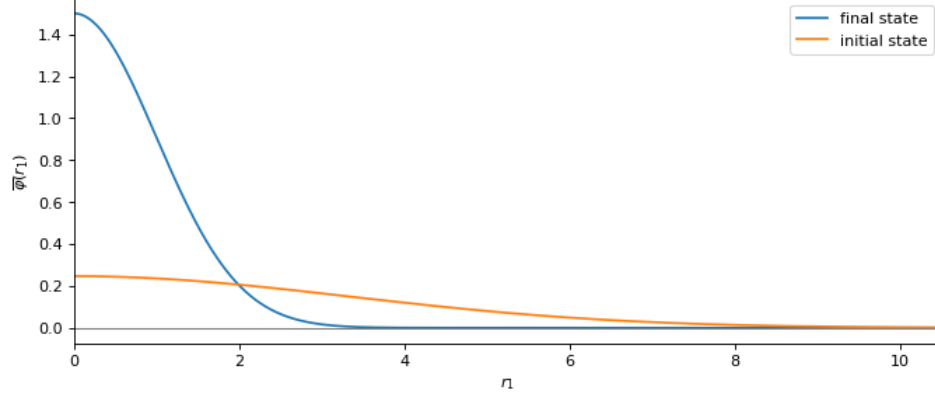

Figure 1: Graphical representation of the free case wave function $\overline{\varphi}(r_1)$ before and after its evolution

From where we can easily identify the initial Gaussian wave function that we are using to start off the evolution with the parameter α set to 1. Our evolution for the free case then, starts off as a Gaussian and it remains a Gaussian throughout the evolution but with a changing parameter that evolves into $\alpha = 1$. This can be visualized in figure 1.

When we calculate the chemical potential and the different energy contributions of the system we find:

μ	E	T	V_h	V_i
1.499967	1.499967	0.748859	0.751108	0.0

Table 2: Table of the chemical potential, the total energy per particle and its kinetic, harmonic and interaction contributions for the non-interacting case.

We can see that the chemical potential is equivalent to the energy per particle. This is due to the fact that since the particles are independent of one another, the energy required to add or remove a particle from the system is the energy of the particle itself, as it does not depend on the N-1 other particles that surround it.
In addition, we can see we recover the result we would expect for the harmonic oscillator in harmonic oscilator units, $E \approx 3/2$, and Virial's Theorem for the harmonic oscilator case is fulfilled, $T \approx V$.

3 Study of the dependence of relevant observables on the number of particles.

In this part we want to calculate the chemical potential, the energy of the system and the kinetic, harmonic and interacting terms contributing to it for a series of experiments. At each experiment the number of particles varies, as well as some of the parameters used in the evolution process, such as the number of steps in the discrete spatial grid or the number of iterations used to reach the final state.
The parameters used for each experiment, as well as the results for each one are the following:

Experiment	N	μ	E	T	V_h	V_i
1	1000000	42.119	30.120	0.061	18.060	11.999
2	10000	6.866	5.042	0.240	2.977	1.824
3	100000	16.847	12.104	0.124	7.238	4.743
4	1000	3.044	2.425	0.437	1.367	0.620
5	100	1.787	1.652	0.656	0.860	0.136

Table 3: Table of the chemical potential, the total energy per particle and its kinetic, harmonic and interaction contributions for each experiment with number of particles N.

From the table of results we can see the energy of the system grows with the number of particles. This is something to expect since the interaction term is proportional to N, and E must therefore grow with it. The growth in the chemical potential can also be explained by the interacting term: as the interaction increases with N, so does the effect one particle has in the system. The energy necessary to extract one particle becomes then bigger as the number of particle (and the interactions between them) does.

The harmonic term also increase with the number of particles. This is related to the fact that the "width" of our condensate grows with N: as N increases, the probability density becomes "wider", and we have more probabilities of finding a particle in larger values of r (we will see this later when we plot the density probability for different N). Since the harmonic term depends on r, it must grow when r does. Finally we can also see that the kinetic term gets

smaller as N grows, this being consistent with the fact that as the interaction increases, the movement of the particles is reduced. It can also be explained by using the density profiles, shown in section 5. As the density profile gets wider with N, the fourier transform in momentum space gets thinner, reducing the momenta of the particles

4   Thomas-Fermi approximation.

We will now study the behaviour of our Bose Einstein Condensate when we apply the Thomas-Fermi approximation. When we remove the kinetic term, we get that

$$\bar{\mu}\overline{\phi}(r_1) = \left[\frac{1}{2}r_1^2 + \bar{a}_s N |\overline{\phi}(r_1)|^2\right] \overline{\phi}(r_1). \tag{5}$$

If we look now at the table of values for the TF approximation, we will see that the kinetic contribution has obviously become 0, and that the qualitative behaviour of the other terms is more or less similar to the one we had seen before. Nevertheless, when comparing both tables, we can check that for $N = 10^6$ the energy term is almost the same, while for $N = 100$ it has differed.

As we had seen before, the kinetic term is less relevant as N increases and therefore, the TF aproximation becomes more accurate as the number of particles gets bigger.

Experiment	N	μ	E	T	V_h	V_i
1	1000000.000	42.424	30.073	0	17.723	12.350
2	10000.000	6.692	4.764	0	2.836	1.928
3	100000.000	16.748	11.964	0	7.180	4.784
4	1000.000	2.647	1.897	0	1.147	0.750
5	100.000	1.045	0.759	0	0.472	0.286

Table 4: Table of the chemical potential, the total energy per particle and its kinetic, harmonic and interaction contributions for each experiment with number of particles N using the TF approximation. It can be seen the kinetic term is null for every experiment.

5   Density profiles

Having compared the values for the energy, chemical potential, etc. for the GP solution and the TF approximation, we show the density profiles for the experiments $N = 1000$ and $N = 10^6$ in figure 2. For the GP solution, we have
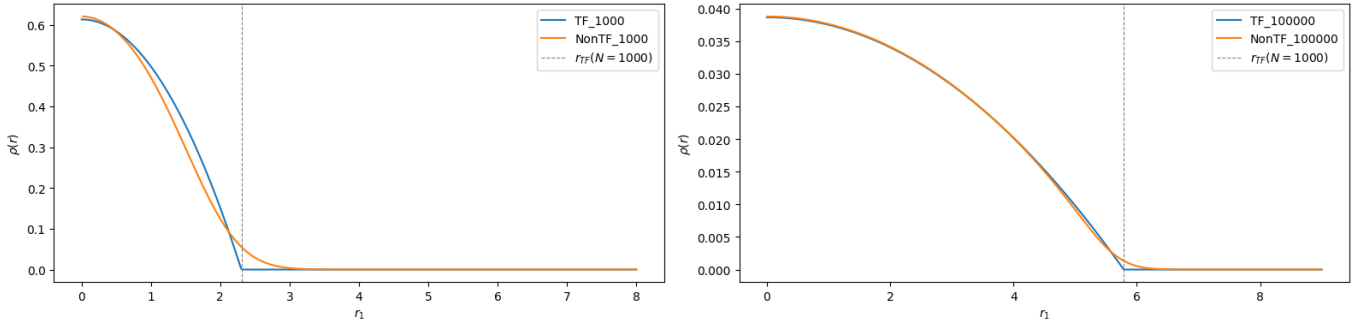
Figure 2: Graphical representation of the density profiles $\rho(r_1)$ for $N = 1000, N = 100000$. In the figure are plotted the density profiles both for the TF approximation and for the GP solution. It can be seen that at $r_{TF}(N)$ the TF density profiles become zero.

used the evoluted radial wave function to calculate the radial density $\rho(r_1) = |\overline{\varphi}(r_1)|^2$. On the other hand, since the kinetic term is removed, the calculus for the TF approximation can be done analytically

$$\bar{\mu} = \frac{1}{2}r_1^2 + \bar{a}_s N|\overline{\varphi}(r_1)|^2 \rightarrow \rho(r_1)_{TF} = \frac{1}{\bar{a}_s N}\left(\bar{\mu} - \frac{1}{2}r_1^2\right). \tag{6}$$

Where expression (6) imposes a maximum radius for TF, such that $r_{TM} = \sqrt{2\bar{\mu}}$. Imposing the normalization of the wave function, we finally find that

$$r_{TM} = (15\bar{a}_s N)^{\frac{1}{5}} \quad \bar{\mu} = \frac{1}{2}(15\bar{a}_s N)^{\frac{2}{5}}$$

From these profiles we can see that the TF approximation improves as N increases like we expected. The density profiles get almost identical as N increases - except for r near r_{TF} -, while for a small N there exists an appreciable variation between both profiles up to r_{TM} approximately, where both tend to 0.

Also, as we had said in section 3, we can see how the Bose-Einstein expands with increasing N resulting in a wider distribution.

6 Virial Theorem

Lastly, we will check the accuracy with which the Virial Theorem is fulfilled. For our Bose Einstein condensate, Virial Theorem tells us:

$$2e_{kin} - 2e_{ho} + 3e_{int} = 0. \tag{7}$$

In the next table we have calculated $2e_{kin} - 2e_{ho} + 3e_{int}$ for every experiment with the results found in b).

Experiment	N	$2T + 3V_i - 2V_h$
1	1000000	-0.000320
2	10000	0.000008
3	100000	0.000004
4	1000	0.000040
5	100	0.000036

Table 5: Check of the accuracy with which the Virial Theorem is fulfilled depending on the number of particles N. The closer the result of $2T + 3V_i - 2V_h$ is to 0, the more accurate.

And in general we see that Virial's theorem is more or less checked for all 5 experiments, this being a good sign of having reached the actual ground state of the system.