

# Numerical methods for resolving the Gross-Pitaevskii equation

Author: Kim Anh Stoeffler

*Facultat de Física, Universitat de Barcelona, Diagonal 645, 08028 Barcelona, Spain.*

Advisor: Bruno Julia Diaz

(Dated: September 2, 2021)

This paper aims at treating the dynamics of a Bose-Einstein condensate at zero temperature, starting from the time-dependant Gross-Pitaevskii equation also known as nonlinear Schrödinger equation. In order to do so, two numerical methods are implemented and studied, in both cases of interacting and non-interacting particles.

## I. INTRODUCTION

For a Bose-Einstein condensate to form, a gas of particles is cooled to a temperature of nearly absolute zero. The transition to the BEC state is set by the condition of quantum degeneracy [1]. Such an "operation" results into a decrease in energy and thus an increase in the particles wavelength [2]. When the temperature is low enough, the wavelengths are larger than the atomic separation, eventually resulting in the creation of a single quantum entity described as a single wave-function. Equivalently, this happens when a fundamental quantum cell of size of the order of de Broglie wave length contains more than one particle. Thus, Bose-Einstein condensates allow the observation of quantum effects on a macroscopic scale and lead to interesting applications in various fields such as transport and conductivity, superfluidity and quantum tunneling [1].

To achieve such a state of matter, the most common techniques are laser cooling and magnetic trapping [3]. If an atomic beam travels in the direction opposite to that of a resonant laser, the beam can be slowed down with a remarkably large deceleration. The velocity spread of the atoms can be dramatically reduced to temperatures in the  $\mu\text{K}$  range above absolute zero [4]. Magnetic fields are used to concentrate and trap atoms into small volumes. Nowadays, one of the most promising developments is the creation of perfectly controlled crystals of atoms loading a Bose-Einstein condensate in a lattice. Those lattices, whose parameters can be varied, form powerful model systems for theory [4].

This paper aims at resolving 2 for both cases  $U_0 = 0$  and  $U_0 \neq 0$  in a one-dimensional system, using the Crank-Nicholson and the imaginary time numerical method. More particularly, the evolution of different initial states in a harmonical trapping potential will be studied for interacting and non-interacting particles.

## II. THEORETICAL APPROACH

### A. The Gross-Pitaevskii equation

In dilute gases, the typical atomic separation isn't small enough for atoms to interact at a significant level

[5]. When distances between particles reduce, it is often convenient to introduce an effective interaction,  $U_0$ . In order to describe interactions between very-long-wavelength excitations and at low energies,  $U_0$  can be taken as a constant in momentum space :

$$U_0 = \frac{4\pi\hbar^2 a}{m} \quad [5] \quad (1)$$

where  $a$  is called the scattering length and characterises the strength of the interactions. In coordinate space, it is given by  $U_0\delta(\mathbf{r} - \mathbf{r}')$  and describes a contact interaction between particles positioned at  $\mathbf{r}$  and  $\mathbf{r}'$  respectively.

The many-particle system can be reduced to the problem of finding a single particle, or condensate wave-function. To describe its time-dependant behaviour, one relies on the Gross-Pitaevskii equation [6], also referred to as the non-linear Schrödinger's equation:

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = \left( -\frac{\hbar^2 \nabla^2}{2m} + V_{ext}(\mathbf{r})(\mathbf{r}, t) + U_0 |\Psi(\mathbf{r}, t)|^2 \right) \Psi(\mathbf{r}, t), \quad (2)$$

where  $\Psi(\mathbf{r}, t)$  is the order parameter or wave function of the condensate.

### B. The Thomas-Fermi approximation

The Thomas-Fermi approximation is a tool which may be used to simplify the Gross-Pitaevskii equation in presence of a trapping potential. The approximation is based on the following physical phenomena : in a trap, both the kinetic energy and interaction energy per particle work to expand the characteristic length of the wave. Hence, one can try to neglect the weaker of the two [7].

Starting from the time-independent one-dimensional Gross-Pitaevskii equation, written as :

$$\left( -\frac{\hbar^2 \partial_x^2}{2m} + V_{ext}(x) + U_0 |\Psi|^2 \right) \Psi = \mu \Psi, \quad (3)$$

where  $\mu$  corresponds to the chemical potential, one can neglect the kinetic energy term when the interaction is

much larger, i.e. for large  $U_0$ .

If one considers a harmonic trapping potential  $V(x) = \frac{1}{2}m\omega^2x^2$ , it is convenient to write the equations using harmonic oscillator units :

$$\bar{t} = \frac{t}{t_{ho}} \quad \bar{\mu} = \frac{\mu}{e_{ho}} \quad \bar{x} = \frac{x}{a_{ho}} \quad \bar{U}_0 = \frac{U_0}{e_{ho}a_{ho}},$$

where  $e_{ho} = \hbar\omega$ ,  $a_{ho} = \sqrt{\hbar/m\omega}$  and  $t_{ho} = \omega^{-1}$ . From now on, every parameter introduced is to be understood in terms of the redefined units. The Thomas-Fermi approximation yields :

$$\left( \frac{1}{2}\bar{x}^2 + \bar{U}_0|\Psi|^2 \right) \Psi = \bar{\mu}\Psi. \quad (4)$$

Resolving Equation 4 leads to the following wavefunction :

$$\Psi_{TF}(x) = \begin{cases} \sqrt{m\bar{\mu} - \frac{1}{2}x^2} & |\bar{x}| < \sqrt{2\bar{\mu}} \\ 0 & |\bar{x}| > \sqrt{2\bar{\mu}}. \end{cases}$$

Normalizing yields  $\bar{\mu} = (3\bar{U}_0/4\sqrt{2})^{2/3}$ .

### C. Solitons

The time-dependent Gross-Pitaevskii equation (2) has exact one-dimensional solutions in the non-linear regime : solitons. These disturbances are wave packets which propagate without any deformation in a non linear dispersive medium. Solitons preserve their form because effects non-linearity compensate those of dispersion. Different types of solitons exist, amongst which one can cite dark solitons. Corresponding to density depressions or holes in the Bose-Einstein condensate, they may be interpreted as a lack of matter.

## III. NUMERICAL APPROACH

The numerical method implemented are the Crank-Nicholson algorithm and the imaginary time method. Both will be discussed and analysed.

### A. Dipolar mode with and without interaction.

The goal of this section is to study the evolution of a particle trapped into a harmonic oscillator when Equation (2) reduces to Schrödinger's equation, i.e.  $g = 0$  and to compare the results when adding a weak interaction between particles. This also allows one to ensure the correct behaviour of the Crank-Nicholson

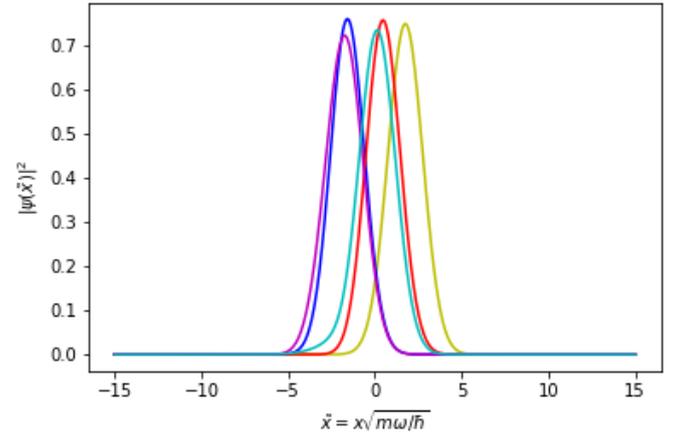


FIG. 1:  $|\Psi(x)|^2$  plotted for different times for the harmonic oscillator case. Yellow curve :  $t= 0.55$  s, blue curve :  $t= 2.55$  s, red curve :  $t= 5.05$  s, magenta curve :  $t= 10.05$  s, cyan curve :  $t= 17.55$  s.

algorithm.

For the sake of simplicity, the particle's mass  $m$  and the constant  $k$  intervening in the potential energy are taken to be equal to 1. The standard deviation  $\sigma$  is similarly set to unity.

Figure 1 depicts the probability density  $|\psi(x)|^2$  at various times. The evolution is expected to maintain the shape of the wave packet : see Figures 2 and 3, respectively illustrating the average position and its incertitude as a function of time.

As one would expect from a particle in a harmonic trap, Figure 1 shows the probability density moving along the  $x$  axis in a back and forth movement. The algorithm preserves the norm as expected : plotted as a function of time, it shows variations of order  $10^{-14}$ .

Plotting the average value of  $x$ , see Figure 2, one may notice constant oscillations corresponding to the back and forth movement of a particle evolving in a harmonic trap. This is verified for both cases of interacting and non-interacting particles. When  $U_0 = 0$ , one may verify that the movement's frequency is in adequacy with the one of the oscillator  $f_{ho}$  :

$$f_{ho} = \frac{\omega}{2\pi}, \quad \omega = \sqrt{\frac{k}{m}} = 1.$$

The oscillations frequency can be derived using a linear interpolation, giving  $f = 0.15734 \simeq \frac{1}{2\pi}$ . However, one would expect the incertitude on  $x$  to be constant, which is not the result depicted by Figure 3. Nonetheless, the oscillating pattern with amplitude growing with time suggest the result is due to the numerical method itself, rather than the physics implemented. A more precise result could be achieved by using a finer space and

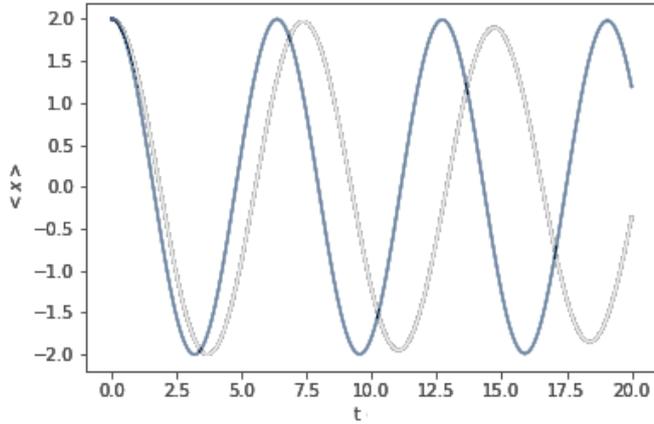


FIG. 2:  $\langle x \rangle$  plotted as a function of time for non interacting (blue curve) and interacting particles (grey) in the harmonic oscillator case in real time evolution.

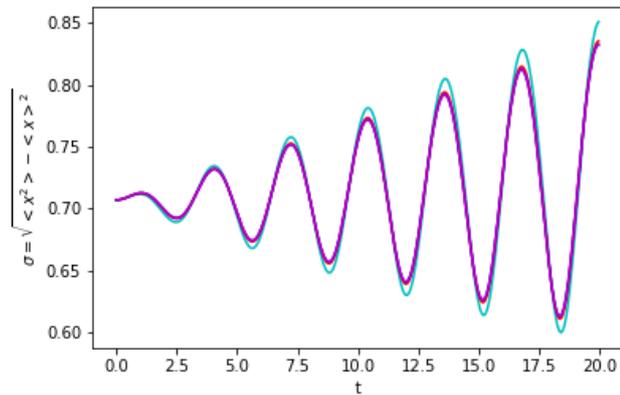


FIG. 3: Uncertainty on  $x$  plotted as a function of time for different number of points in the case of the harmonic oscillator. Cyan :  $N = 400$ , red :  $N = 1000$ , blue :  $N = 5000$  and magenta  $N = 10000$ .

time discretization. Figure 3 corroborates this hypothesis : by implementing a smaller  $\Delta x$  for the spatial grid, one notices the oscillations of  $\sigma$  diminishing.

The norm is still conserved by the algorithm and the density evolves as expected when adding an interaction of amplitude  $U_0 = 1$ . The results are quite similar to the ones obtained in the previous section : in fact, the dipolar mode should be independent of the interaction. Overall, the results obtained are satisfying and suggest the Crank-Nicholson numerical method is a good approach to solving the Gross-Pitaevskii equation.

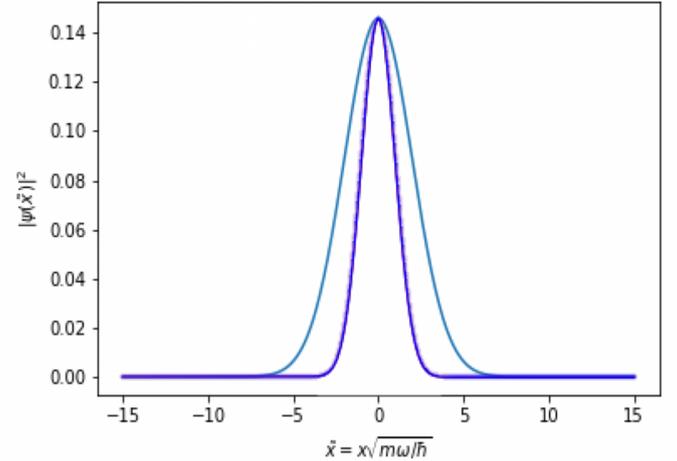


FIG. 4: Initial condition implemented for the imaginary time propagation (case  $U_0 = 0$  and  $V_{ext} \propto x^2$ ) and comparison between the plot of the evolved state obtained with the IPT method and the plot of the system's ground state.  $\sigma = 2$ .

#### IV. IMAGINARY TIME

This section aims at resolving the GP equation (for  $U_0 = 0$  and  $U_0 \neq 0$ ) making use of the imaginary time propagation (IPT) numerical method. The latter consists into replacing the time  $t$  by an imaginary time, introducing  $\tau$  such that  $t = -i\tau$ . The formal solution of the GP equation is hence given by the evolution operator  $\exp(-\tau H)$ , with  $H$  being the system's Hamiltonian. Any initial condition is hence meant to converge asymptotically to the ground state solution for  $\tau$  large enough. In what follows, the initial conditions implemented are taken amongst a Gaussian, the Thomas-Fermi wave-function or an orthogonal state to the Gaussian defined as :

$$\Psi(x) = \frac{1}{\sigma\pi^{1/4}} \exp\left(\frac{-(x-\mu)^2}{2\sigma^2}\right). \quad (5)$$

##### A. Harmonic oscillator case ( $U_0 = 0$ and $V_{ext} \propto x^2$ )

In this section, the initial condition is taken to be a centred Gaussian of width  $\sigma = 2$  (see Figure 4). One thus expects to obtain a Gaussian of width  $\sigma = 1$  after running the simulation.

Figure 4 confirm that the state obtained with the ITP method is, as expected, the ground state of the harmonic oscillator. In fact, the curve obtained by running the numerical algorithm is perfectly superposed to the one corresponding to the theoretical ground state. One may also verify the energy of the state obtained coincides with the theoretical one : computing numerically the energy using the trapezoidal method, one obtains a value of

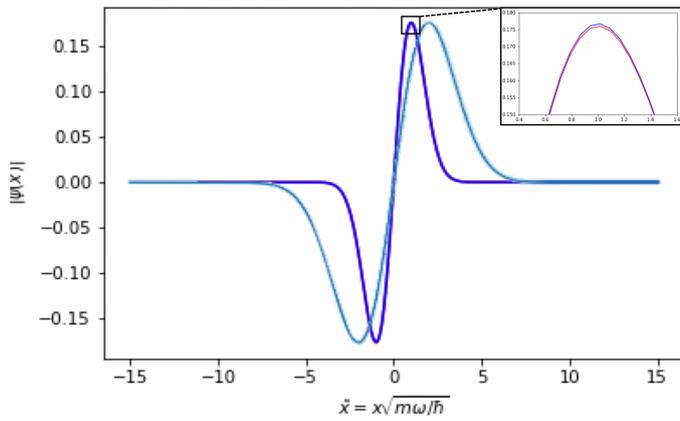


FIG. 5: Initial condition (5) implemented for the imaginary time propagation and comparison between the plot of the evolved state obtained with the IPT method and the plot of the system's first excited state (case  $U_0 = 0$  and  $V_{ext} \propto x^2$ ).

$E_0 = 0.54$ . This in fact corresponds to the expected result for the ground state of the harmonic oscillator since  $E_{0,th} = \frac{\hbar\omega}{2} = 0.5$  when  $\hbar = \omega = 1$ .

The same study may be lead implementing as initial condition a wave function orthogonal to the ground state. In this case, one expects to obtain the first excited state of the harmonic oscillator.

Once again, Figure 5 suggest the algorithm in fact leads to the expected state with a good precision. Computing the energy of the state obtained, one finds a value of  $E_1 = 1.499$ , which is the expected result for the first excited state of the harmonic oscillator. The method could be improved by a finer discretization of time and/or space.

### B. With an effective interaction $U_0 = 50$

In this section, the imaginary time method is used to evolve various initial states when considering the Hamiltonian of many bodies, when particles are trapped in a harmonic oscillator potential. In a first approach, a Gaussian is plotted as the initial state : see the light blue curve of Figure 4.

The results being highly sensitive to time discretization, the simulations are run with a time interval  $dt = 0.01$ . There is however a noticeable difference between the Thomas Fermi state and the ground state obtained with the imaginary time evolution. This may be explained by the approximations used on both sides. The numerical method first of all introduces errors at each time step as it is not an exact resolution of GP equation. On the other hand, the Thomas Fermi limit is itself an approximation of the initial problem, hence explaining the differences observed. The approximation is expected to be more accurate for a higher interaction between particles.

Starting from an orthogonal state, for example the

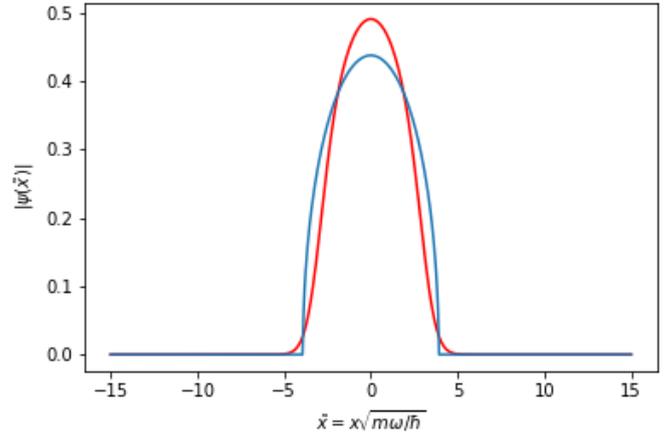


FIG. 6: Comparison between the plot of the evolved state obtained with the IPT method (red) and the plot of the state corresponding to the Thomas Fermi approximation (blue) with a time interval  $dt = 0.01$  (case  $U_0 = 50$ ).

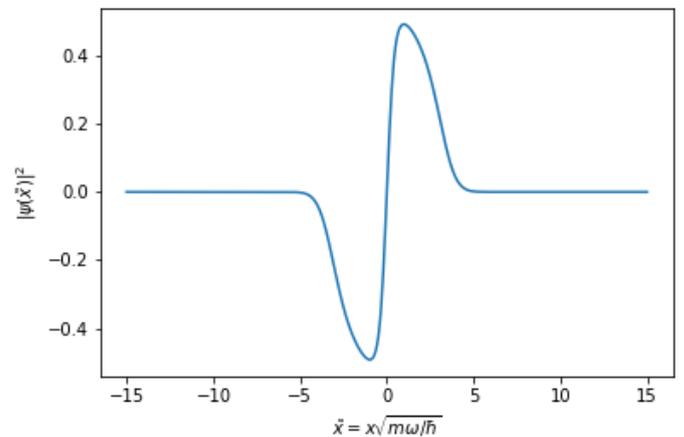


FIG. 7: 1st excited state obtained with the imaginary time method when  $U_0 = 50$  for an initial condition given by Equation (5).

wave-function given by Equation 5, one obtains the first excited state as shown by Figure 7. Figure 8 depicts the real time evolution of the first excited state, the different colours corresponding to various moments in time. The energy is similarly expected to converge towards a certain value : this result is depicted by Figure 9.

The imaginary time method can yield a quasi-stationary state with a displaced soliton (see Figure 11). This is achieved running the imaginary time method with the following initial state :

$$\psi_0(x, d) = \psi_{TF}(x) \tanh(x - d) \quad (6)$$

where  $\psi_{TF}(x)$  designates the wave-function of the Thomas-Fermi approximation and  $d$  is a displacement

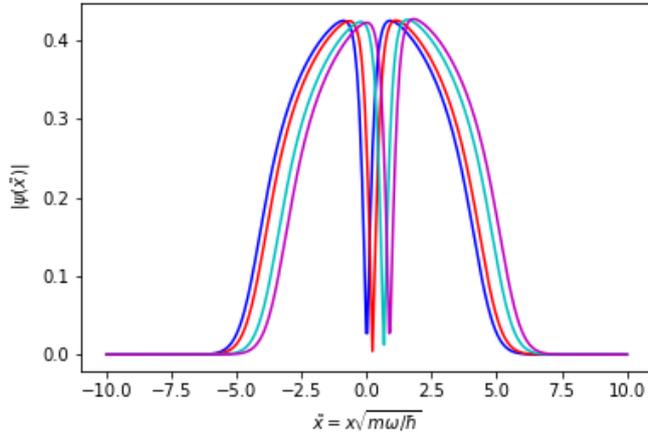


FIG. 8: Real time evolution of the 1st excited state obtained with the imaginary time method for  $U_0 = 50$ .

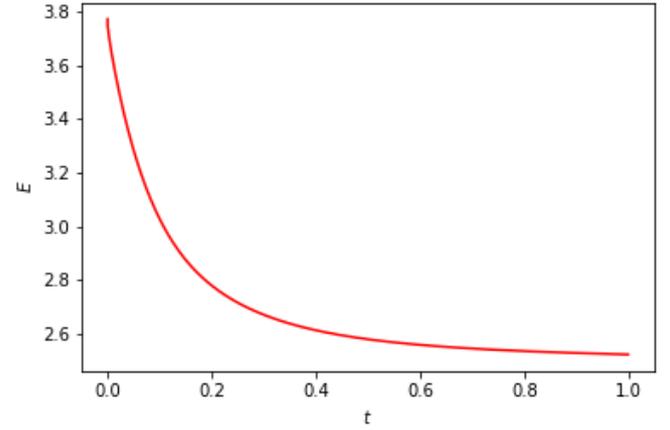


FIG. 10: Energy convergence of the imaginary time evolution when starting with a dark solitonic state, see Equation (6), and for a perturbation  $U_0 = 50$ .

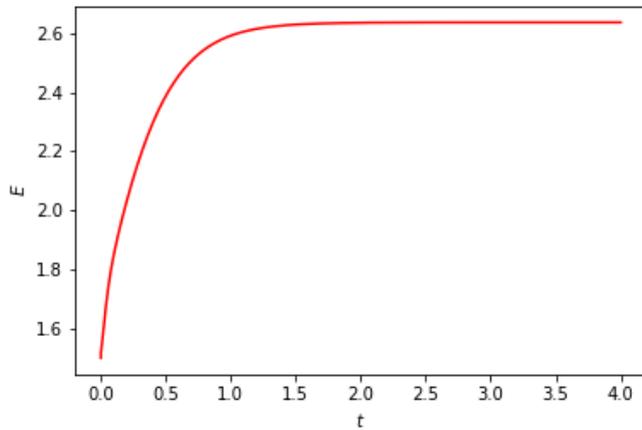


FIG. 9: Energy convergence of the imaginary time method for  $U_0 = 50$  and an initial state given by (5).

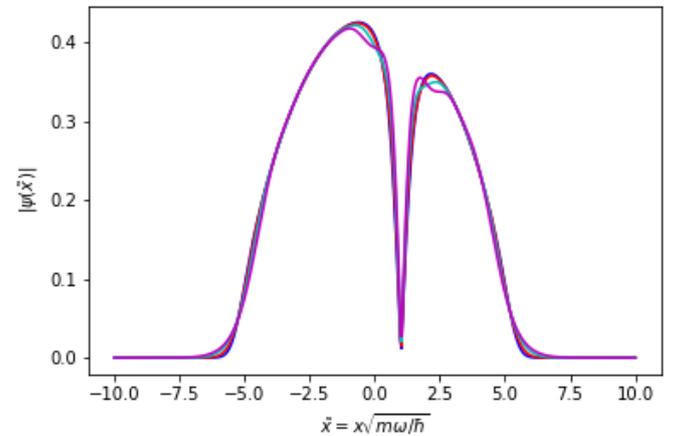


FIG. 11: Imaginary time evolution of a dark solitonic state (6) for  $U_0 = 50$ .

from the origin. Figure 11 in fact depicts very slight differences between the solitonic state at different times. The plot of the energy, see Figure 10, shows the quick convergence of the energy towards a stable plateau.

and time. A solitonic state has been achieved using the imaginary time method.

## V. CONCLUSION

The studies conducted have shown the the efficiency of the Crank-Nicholson method and the imaginary time algorithm to resolve the linear and non-linear Schrödinger's equation. In fact, the results appeared to be in general accuracy with what was expected. The Thomas-Fermi approximation turned out to be a good approach to resolving the GP equation. However, the approximation could have been more accurate with a higher interaction term between particles and a finer discretization of space

## VI. PERSONAL EXPERIENCE

Working on this project with Prof. Bruno Julia has been a rewarding experience. I learned to code in Python (previously using c++), a language which turned out to be very useful and convenient. Tackling the very interesting subject of Bose-Einstein condensates taught me a lot, both on academic and personal point of views. In fact, it allowed me to dig deeper into applied physics in a branch I was already interested in. Hence, I aim at continuing my studies in similar fields.

Working on this project was not always easy considering the 4 other subjects I had taken, most of which were in Catalan, a language I am not familiar with, but it taught me to organise my time wisely. I would have enjoyed something with more of human contact and less screen

time, but the Covid pandemic unfortunately didn't allow it. Another difficulty I faced, again due to the sanitary situation, is the fact that I barely got to meet any of my classmates. I hence was working and studying by myself during the whole semester. Although it has its downsides (such as losing a lot of time trying to figure everything out on my own), this situation helped me rely more on myself and trust my abilities.

Overall, working on this project gave me a clearer view on how a scientific report is constructed and what is expected from a physicist. It taught me to have certain reflexes in order to lead fine and rigorous analysis. I most definitely enjoyed the project and I am more than happy to have done it. Prof. Bruno Julia was very helpful and understanding along with being a great teacher which made my experience quite pleasing.

- 
- [1] C S Unnikrishnan, *Bose-Einstein Condensates as Universal Quantum Matter*, 2018. hal-01949624
  - [2] Mariusz Gajda, Kazimierz Rzazewski-*Fluctuations of Bose-Einstein condensate*, Phys. Rev. Lett. 78, 2686 - Published 7 April 1997
  - [3] C.J. Pethick, H. Smith - *Bose-Einstein condensation in Dilute Gases*
  - [4] Michèle Leduc, Julien Dugué, Juliette Simonet, *AIP Conference Proceedings 1119, 37*, Published Online: 29 April 2009
  - [5] Frédéric Mila - *Physique statistique 1*, EPFL
  - [6] Lev Pitaevskii, Sandro Stringari - *Bose Einstein condensation*
  - [7] Yves Castin, ENS - *Mécanique quantique : Seconde quantification et résolvente*, retrieved from <http://www.phys.ens.fr/~castin/cours.pdf>
  - [8] A. R. Fritsch, Mingwu Lu, G. H. Reid, A. M. Piñeiro, I. B. Spielman - *Creating solitons with controllable and near-zero velocity in Bose-Einstein condensates*