Properties of Bose-Einstein Condensates in a mean-field description

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Abstract: We study the properties of Bose-Einstein Condensates in a harmonic trap. We consider a mean-field description in terms of the Gross-Pitaevskii equation. We study properties of its solutions, especially the ground state of the system, paying a special attention to the effects of interaction. To obtain numerically the exact stationary states we use the Crank-Nicholson Scheme.

I. INTRODUCTION

The Bose-Einstein condensate is a quantum phenomenon predicted by Einstein in 1925 based on a paper from Bose. It was first observed in 1995 and for this reason, later in 2001 Eric A. Cornell, W. Ketterle and C. E. Wieman received the Nobel Prize. An extended historical introduction can be found in Ref. [1].

When a number of bosons are trapped by an external potential at very low temperature, most of the particles condense in the same single particle ground state. Therefore we can describe the microscopic behavior of the system with a single wave-function. This is called the Bose-Einstein condensate (BEC).

There are two potential terms to consider. First, we have an external harmonic potential which keeps the atoms localized in space. Secondly, we have an interaction term due to the atom-atom interaction. We study the whole system in a mean-field theory for a diluted condensate. In these conditions the equation which describes the condensate is the Gross-Pitaevskii equation. We restrict this work to a one-dimensional problem, this is experimentally possible by using a much higher trapping frequency in a plane than in the direction we will study. This effectively freezes the dynamics on the transversal plane leaving only one free direction.

We follow the next scheme. First, in Sec. II we explain the theoretical background and the external conditions that we impose. In Sec. III we discuss the Crank-Nicholson method and its applicability in the Gross-Pitaevskii equation. We also show a way to compute stationary states of the system, especially the ground state, which consist on performing an imaginary time evolution instead of real time. In Sec. IV we study the equation without interaction. We characterize the ground and first excited state and temporal evolution. In Sec. V we include the interaction and again characterize the ground state and compare it with the Thomas-Fermi limit, in which the kinetic term is neglected

II. THEORETICAL BACKGROUND

A. Gross-Pitaevskii equation

We consider N bosons trapped by a harmonic trap $V = \frac{1}{2}m\omega^2 x^2$ at low temperatures, ideally zero.

For simplicity we will write all magnitudes in terms of the following harmonic oscillator natural units. For energy the unit is $E_0 = \hbar\omega$, space $a_0 = \sqrt{\frac{\hbar}{m\omega}}$ and time $t_0 = \omega^{-1}$.

We consider an effective repulsive contact atom-atom interaction to describe the atomic collisions. Which is a reasonable approximation for diluted gases. The expression of the internal potential is $V_{int} = g_{1D}N\delta(x_i - x_j)$.

Assuming the many-body wave-function can be written as $\psi(x_1, ..., x_n) = \prod_{i=1}^{n}\varphi(x_i)$, Gross and Pitaevskii derived in the mean-field approximation the following equation,

$$\begin{aligned} i\frac{\partial\varphi(x,t)}{\partial t} &= -\frac{1}{2}\frac{\partial^2\varphi(x,t)}{\partial x^2} + V(x)\varphi(x,t) \\ &+ g_{1D}N|\varphi(x,t)|^2\varphi(x,t). \end{aligned} \tag{1}$$

The procedure to obtain this equation can be found in Ref. [2]. Note this equation has several terms which are similar to the Schrödinger equation. The second term is the external potential,

$$V(x) = \frac{1}{2}x^2. \tag{2}$$

The last term is the interaction potential and breaks the linearity of the equation. The constant g_{1D} gives the intensity of the interaction and is the relevant parameter. The total energy is calculated with the following formula [2],

$$\begin{aligned} E &= \frac{1}{2}\int_{-\infty}^{\infty}(-\varphi^*(x,t)\frac{\partial^2\varphi(x,t)}{\partial x^2} + x^2|\varphi(x,t)|^2 \\ &+ g_{1D}N|\varphi(x,t)|^4)dx. \end{aligned} \tag{3}$$

B. Virial Theorem

For the ground state of the Gross-Pitaevskii equation, one can derive the following Virial theorem,

$$2\langle T\rangle - 2\langle V\rangle + \langle V_{int}\rangle = 0. \tag{4}$$

Where $\langle T\rangle$, $\langle V\rangle$ and $\langle V_{int}\rangle$ are the expectation values of kinetic, harmonic oscillator potential and interaction potential energy, respectively. In this relation we see that if the interaction is zero we recover the Virial theorem for the harmonic oscillator $\langle T\rangle = \langle V\rangle$.

C. Thomas-Fermi limit

This limit consist on neglecting the kinetic term in the Gross-Pitaevskii equation, this is useful because in many experiments with large number of atoms it gives a very good approximation to the full solution. Also then the solution of the Gross-Pitaevskii equation becomes analytic. Similar calculations and more information are in Ref. [3]. In this situation, the Gross-Pitaevskii equation for stationary states $\varphi(x,t) = \varphi(x)e^{i\mu t}$ becomes,

$$\mu\varphi(x) = V(x)\varphi(x) + g_{1D}N|\varphi(x)|^2\varphi(x). \tag{5}$$

From Eq. (5) and Eq. (2) the probability density is,

$$|\varphi(x)|^2 = \frac{\mu - \frac{1}{2}x^2}{g_{1D}N}. \tag{6}$$

Forcing $|\varphi(x)|^2 \geq 0$ then this function is valid for $-\sqrt{2\mu} \leq x \leq \sqrt{2\mu}$ and zero otherwise. Now to find μ we need to impose normalization $\int_{-\sqrt{2\mu}}^{\sqrt{2\mu}} |\varphi(x,t)|^2 dx = 1$,

$$\mu = \frac{1}{2}\left(\frac{3}{2}g_{1D}N\right)^{2/3}. \tag{7}$$

From the wave-function, an important relation can be readily obtained which provides a simple formula for the size of the BEC in this limit. Let us compute the mean square radius of the atomic cloud,

$$\langle x^2\rangle = \int_{-\sqrt{2\mu}}^{\sqrt{2\mu}} x^2|\varphi(x,t)|^2 dx = \frac{2}{5}\mu. \tag{8}$$

And the total energy using Eq. (3),

$$E = \frac{3}{5}\mu. \tag{9}$$

In Sec. V we will compare these simple expressions with the full numerical solution of Eq. (1).

III. NUMERICAL METHOD: CRANK-NICHOLSON

To solve the Gross-Pitaevskii equation we use the Crank-Nicholson method described in Ref. [4]. We work in a finite box of length equal to $20a_0$, $(-10 > x > 10)$. Using this scheme Eq. (1) becomes,

$$\begin{aligned} i\frac{\varphi_i^{n+1} - \varphi_i^n}{\Delta t} = &-\frac{1}{4\Delta x^2}((\varphi_{i+1}^{n+1} - 2\varphi_i^{n+1} + \varphi_{i-1}^{n+1}) \\ &+ (\varphi_{i+1}^{n} - 2\varphi_i^{n} + \varphi_{i-1}^{n})) + \frac{1}{2}V_i(\varphi_i^{n+1} + \varphi_i^n) \\ &+ \frac{1}{2}g_{1D}N|\varphi_i^n|^2(\varphi_i^{n+1} + \varphi_i^n). \end{aligned} \tag{10}$$

Where the subindex i, refers to space and superindex n, to time $\varphi_i^n = \varphi(i\Delta x, n\Delta t)$. This method makes a temporal average from n and $n+1$, it is centered in $n+\frac{1}{2}$ which allows one to achieve a second order accuracy in time, this is the reason we have chosen this scheme. To solve this system of equations, first we rearrange all these terms,

$$f_i = b\varphi_{i+1}^{n+1} + a_i\varphi_i^{n+1} + c\varphi_{i-1}^{n+1}. \tag{11}$$

Where

$$\begin{aligned} b &= i\frac{\Delta t}{4\Delta x^2}, \qquad c = i\frac{\Delta t}{4\Delta x^2} \\ a_i &= -i\left(\frac{\Delta t}{2\Delta x^2} + \frac{V_i\Delta t}{2} + \frac{1}{2}g_{1D}N|\varphi_i^n|^2\right) - 1 \\ f_i &= -i\left(\frac{\Delta t}{4\Delta x^2}\left(\varphi_{i+1}^n - 2\varphi_i^n + \varphi_{i-1}^n\right) - \frac{V_i\Delta t}{2}\varphi_i^n \right. \\ &\quad \left. -\frac{1}{2}g_{1D}N|\varphi_i^n|^2\varphi_i^n\right) - \varphi_i^n. \end{aligned}$$

We use the Thomas method explained in Appendix A to solve the tridiagonal system of equations. In our program we set a discretization in x of 1000 points which allows us a good description of the wave-function in the trap.

A. Imaginary Time

In this section we introduce a way to find stationary states using the method of imaginary time evolution. From quantum mechanics we know that evolution is ruled by the evolution operator, a unitary operator which for a time-independent Hamiltonian can be written as: $U = e^{\frac{itH}{\hbar}}$, and the evolution of an initial state is $|\varphi(t)\rangle = U|\varphi(0)\rangle$. Now, if we change the parameter t to a pure imaginary time $t = -i\tau$, the operator U is not anymore unitary and this evolution will make the wave-function loose normalization and eventually collapse. But if we normalize the wave-function after every time step, the method will lead the wave-function to the lowest-energy stationary state with a non-zero overlap with the initial state.

This method does not require accuracy on time and therefore we use a large time step ($\Delta t = -i0.01$) to obtain the results in only a few seconds.

B. Real Time

The real-time evolution of an initial wave-function requires larger precision for the method to converge. We have found that we need a step time at most of $\Delta t = 0.0001$ or lower in order to achieve good convergence of the method. Larger values for Δt cause small spurious fluctuations in the wave-function at the first steps and eventually grow to loose the wave-function. Since the time step is so small it takes a few minutes to compute 10 time units. If we neglect the internal interaction term in the Gross-Pitaevskii equation we may increase the time

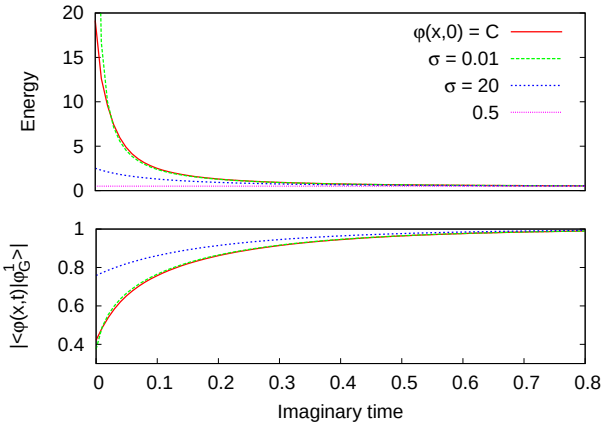

FIG. 1: Evolution of the energy and overlap with the ground state with initial wave-function, $\varphi(x,0) = C$, $\varphi = \varphi_G^\sigma(x)$ with $\sigma = 0.01$ and $\sigma = 20$ as function of the imaginary time.

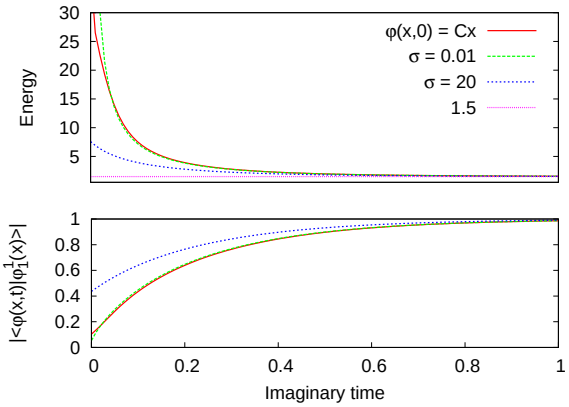

FIG. 2: Evolution of the energy and overlap with the first excited state with initial wave-function, $\varphi(x,0) = Cx$, $\varphi = \varphi_1^\sigma(x)$ with $\sigma = 0.01$ and $\sigma = 20$ as function of the imaginary time.

step by a factor 10 keeping stability in the simulation. This proves that the nonlinear term is a source of numerical instability.

IV. NON-INTERACTING CASE: HARMONIC OSCILLATOR

First we discuss the non-interacting case which is essentially the single particle problem trapped by a harmonic potential. This is also discussed in Ref. [3].

A. Stationary states

The eigenfunctions of the harmonic oscillator are well known, thus we can use them to explore the convergence of the imaginary time method. For the ground state the wave-function takes the form, $\varphi_G^\sigma(x) = \left(\frac{1}{\pi\sigma^2}\right)^{1/4} e^{\frac{-x^2}{2\sigma^2}}$ with $\sigma = 1$.

We consider three different initial wave-functions and study how the methods converge to the exact solution. First, we consider two initial functions, the same expression than the ground state, but with different σ, $\sigma = 0.01$, $\sigma = 20$ and the last one is a constant $\varphi(x,0) = C$. In Fig. 1 we see the evolution of the energy and the overlap with the ground state. As a function of the imaginary time they converge to energy $\frac{1}{2}h\omega$ and overlap equal to 1, does finding the correct result.

Now we do the same for the first excited state where the wave-function is, $\varphi_1^\sigma(x) = \left(\frac{1}{\pi\sigma^2}\right)^{1/4} \sqrt{2}xe^{\frac{-x^2}{2\sigma^2}}$ with $\sigma = 1$. The initial functions are with $\sigma = 0.01$, $\sigma = 20$ and the last one $\varphi(x,0) = Cx$. Note these wave-functions are orthogonal to the ground state but have a non-zero overlap with the first exited state. In Fig. 2 we see that the energy converges to $\frac{3}{2}h\omega$ and the overlap with φ_1^1 state converges to 1, finding again the correct result.

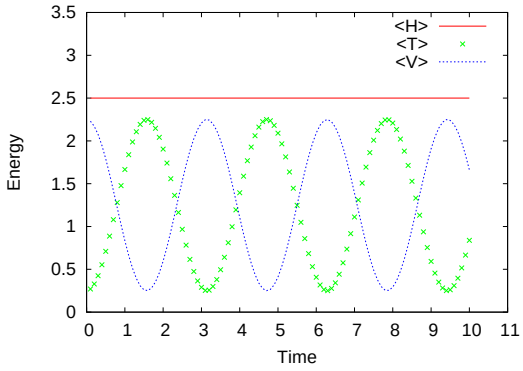

FIG. 3: Evolution of the energy with initial function, $\varphi(x, t = 0) = \varphi_G(x - 2)$.

B. Non-stationary states

Now, we will see the evolution in real time of a non-eigenstate function. Our initial function now is $\varphi(x,0) = \varphi_G(x-2)$. Fig. 3 shows the evolution of the following magnitudes, total energy, kinetic energy and potential energy. The total energy remains constant as expected and the kinetic and potential energies oscillate with the same period but opposite phase.

Fig. 4 shows the evolution of the wave-function at different times. The wave packet oscillates within the harmonic oscillator. As expected, the center of the cloud oscillates in a way similar to the classical oscillation with frequency ω.

V. INTERACTING CASE

Now we study the Gross-Pitaevskii equation including the interaction term. We fix $N = 100$ and vary the interaction strength g_{1D}. This is experimentally possible by

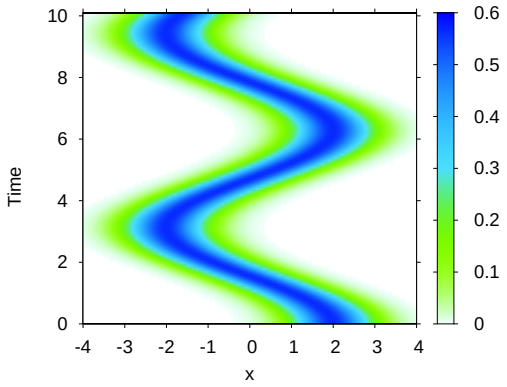

FIG. 4: Evolution of the initial wave-function $\varphi(x,0) = \varphi_G(x-2)$. The color code is $|\varphi(x,t)|^2$.

means of Feshbach resonances discussed in Ref. [5].

A. Ground state properties

We want to study the properties of the ground state. We use, as we did in the previous section, the method of imaginary time. The initial wave-function in this case is $\varphi_G^\sigma(x)$ with $\sigma = 1$, which is the ground state of the harmonic oscillator without interaction. First we prove quantitatively the convergence of the method and verify that Crank-Nicholson can be applied in a non-linear equation as Gross-Pitaevskii equation. For this purpose we rewrite Eq. (1) for stationary states $\varphi(x,t) = \varphi(x)e^{i\mu t}$,

$$\mu(x) = \frac{-\frac{1}{2}\frac{\partial^2\varphi(x,t)}{\partial x^2} + V(x)\varphi(x,t) + g_{1D}N|\varphi(x,t)|^2\varphi(x,t)}{\varphi(x,t)}. \tag{12}$$

Now we have a chemical potential which formally depends on x. A good test of the convergence of the imaginary time evolution is to check that $\mu(x) \simeq \mu$, constant. In Fig. 5 we depict $\mu(x)$ after the imaginary time evolution. Indeed we find a good convergence of the results.

Lets now discuss the properties of the BEC. In Fig. 6 we show the dependence of the properties of the BEC with the parameter $g_{1D}N$. First, we observe that in absence of atom-atom interaction we recover the results discussed in Sec. IVA. On the top panel we show the average value of kinetic, external potential, internal potential and total energy which verifies the Virial Theorem showed in Sec. IIB. We see that increasing g_{1D} makes all energies grow except the kinetic energy which diminishes. In the middle panel we show the mean square radius, this gives a measurement of the size of the BEC which grows with g_{1D}, as expected from a repulsive interaction. The bottom panel shows the chemical potential which also grows with g_{1D}. All these magnitudes are compared with the Thomas-Fermi prediction discussed in Sec. IIC which is

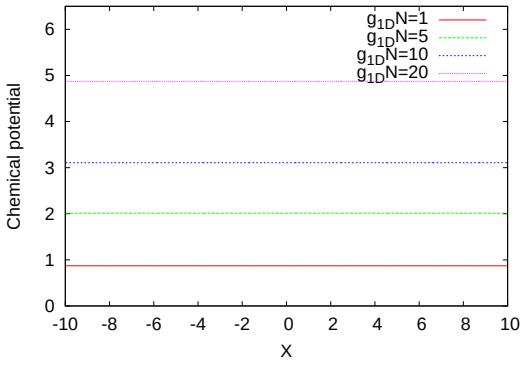

FIG. 5: Chemical potential computed with Eq. (12). The fact that the result is constant in all the domain reflects the convergence of the imaginary time method. The final imaginary time is $\tau = 10$.

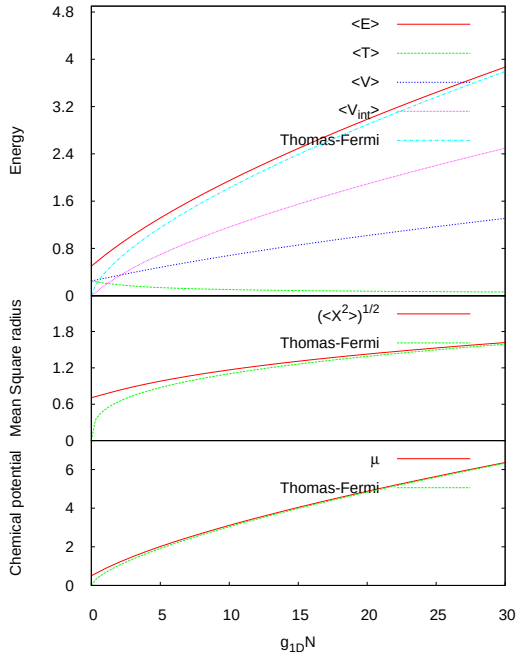

FIG. 6: Variation of energies, mean square radius and chemical potential for the ground state for different values of g_{1D} compared to the Thomas Fermi prediction.

very close to the exact solution for large interaction.

Fig. 7 shows the profiles of the wave-function for different intensities of interaction and compares them with the prediction of the Thomas-Fermi. For low values of g_{1D} the wave-function is similar to the harmonic oscillator ground state and is very different from the Thomas-Fermi prediction. For larger interaction the wave-function becomes wider and it matches the Thomas-Fermi profile only differing in the tails where the kinetic energy is still important.

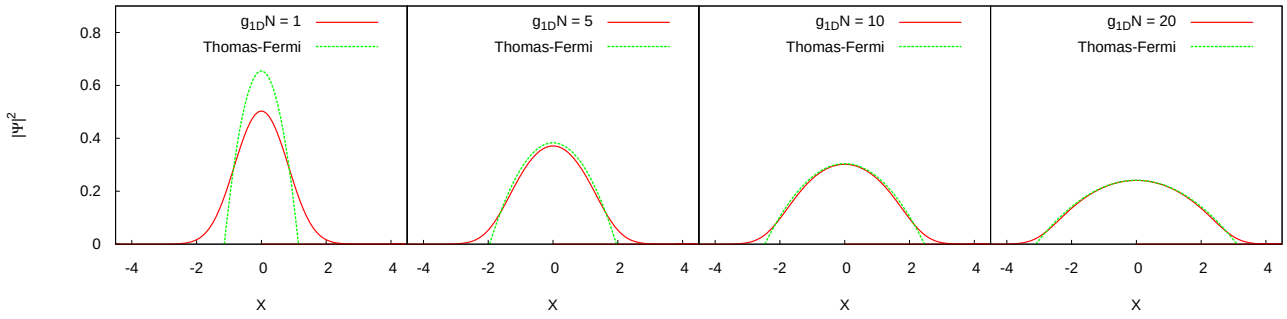

FIG. 7: Profile of the ground state for different values of $g_{1D}N = 1, 5, 10, 20$, compared with the Thomas Fermi prediction.

VI. CONCLUSIONS

We have discussed the properties of Bose-Einstein condensates in mean-field approximation which we described by the Gross-Pitaevskii equation. We used the Crank-Nicholson scheme to numerically obtain the exact solutions of this equation. We proved the convergence of the method and the effectiveness of imaginary time evolution method using the non-interacting case (Sec. IV) and found the well-known harmonic oscillator results.

For the interacting case (Sec. V) we saw that the Crank-Nicholson scheme is valid for this non-linear equation and therefore we have computed the properties of the BEC. We have shown that interaction introduces a non-linear term in the equations which adds numerical instability. We see that interaction makes the BEC grow in size and energy and for large interactions we find that Thomas-Fermi approximation is justified as the exact results match the analytic prediction of this limit.

An interesting next step in this work would be to study the time evolution in the Gross-Pitaevskii equation to obtain the dynamic properties introduced by the interaction.

APPENDIX A: THOMAS METHOD

We use the Thomas algorithm to solve tridiagonal systems of equations detailed in Ref. [6]. Given the system of equations in matrix notation, $T\varphi = f$

$$T = \begin{pmatrix} a_1 & c_1 & & & \\ b_2 & a_2 & c_2 & & \\ & . & . & . & \\ & & . & . & c_{n-1} \\ & & & b_n & a_n \end{pmatrix}. \tag{A1}$$

Where φ is the solution of the system. The matrix T can be decomposed as a product of two different matrices $T = LU$,

$$L = \begin{pmatrix} 1 & & & \\ \beta_2 & 1 & & \\ & . & . & \\ & & \beta_n & 1 \end{pmatrix} U = \begin{pmatrix} \alpha_1 & c_1 & & \\ & \alpha_2 & c_2 & \\ & & . & . \\ & & & \alpha_n \end{pmatrix}. \tag{A2}$$

Now to solve the original system is equivalent to solve the following systems, $Lg = f$ and $U\varphi = g$, but these are much easier to solve. The algorithm to solve the system consist on the following steps;

1) $\alpha_1 = a_1$
2) $\beta_i = \frac{b_i}{\alpha_{i-1}}$; $\alpha_i = a_i - \beta_i c_{i-1}$, $i = 2, 3, ..., n$
3) $g_1 = f_1$
4) $g_i = f_i - \beta_i g_{i-1}$, $i = 2, 3, ..., n$
5) $\varphi_n = \frac{g_n}{\alpha_n}$
6) $\varphi_i = \frac{g_i - c_i \varphi_{i+1}}{\alpha_i}$, $i = n-1, n-2, ..., 1$.

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