Bright soliton dynamics in confining and expelling potentials

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Abstract: This work presents an exploration of the dynamics of a Bose-Einstein Condensate (BEC) with a focus the bright soliton solution for the 1D Gross-Pitaevskii equation. The Crank-Nicolson algorithm is used to study the soliton trapped in a harmonic oscillator potential well, a case which can be used to test the solver. Two vibration modalities are revealed: Oscillations, with frequency $\omega_{osc} = \omega$, and squeezing, with $\omega_{sq} = 1 + 0.055 \times \xi^{-2.49}$. Then the soliton is placed in an inverted harmonic oscillator potential, on which different dynamical regimes are discussed, which depend on the healing length and the oscillator length scale, presenting a transition at $\xi \approx 0.30 \pm 0.05 a_0$.

I. INTRODUCTION: THE BOSE EINSTEIN CONDENSATE

When a sample of atoms or subatomic particles in the form of gas is cooled down to near absolute zero, it may coalesce into a single quantum entity. That is, all their particles can be described as a single wave function, even at a near macroscopic scale [1]. This form of matter is what we call a Bose-Einstein Condensate (BEC), and was predicted to exist by Albert Einstein in 1924 [2].

However, this behaviour was not proven until many years after (in the 2000s), when united states physicists Eric A. Cornell and Carl E. Wieman, as well as german physicist Wolfgang Ketterle received a Nobel Price for synthesizing the first case of this new state of matter [3].

This work will cover the dynamics of a BEC under a specific set of conditions, and ultimately simulate how a soliton configuration of such gas falls and/or breaks apart when subjected to an inverted harmonic potential. To do so, this work is organized as follows: Section II exhibits the Gross-Pitaevskii equation, the one most used to study BECs, as well as introduces the analytical solutions that will be worked on for the rest of the work. After that, in section III a harmonic potential is included into the equation and a new set of units is defined. Section IV explains the numerical solvers used for simulating the BEC, as well as briefly discusses the software developed during the making of this work. Then, sections V and VI explore the simulation results of a soliton both oscillating in a harmonic oscillator, and falling off of an inverted one. Finally, section VII provides a conclusion for the work.

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II. THE GROSS-PITAEVSKII EQUATION

When solving for a BEC's wave function, assuming a mean-field description for the bosonic gas, its dynamical can be described with the time dependent Gross Pitaevskii equation, a nonlinear extension of the Schrödinger equation, which reads [4] [5] [6]

$$i\hbar \frac{\partial \psi(\mathbf{r})}{\partial t} = \left(-\frac{\hbar^2 \nabla^2}{2m} + V(\mathbf{r}) + gN \left| \psi(\mathbf{r}) \right|^2 \right) \psi(\mathbf{r}), \quad (1)$$

where m is the mass of the bosons being described, V is an external potential, g represents the strength of the inter-particle interaction, and N is the number of particles. Keep in mind that this equation is only valid for condensates in fairly strict conditions, such as them being at ultracold temperatures.

Let us introduce a new set of constants: ξ will be the healing length of a soliton, which will characterize the distance at which the soliton, when disturbed, will return to its original shape (A soliton refers to a solution of the GP equation, the density profile of which does not change during its evolution when free from an external potential). c will be the speed of sound in the BEC, n will be considered to be the density of the solution ($|\psi|^2$), whereas n_i will refer to this same density on a specific place of our solution (n_∞ is the background density of the BEC, whereas n_0 is the central density) [6]. ξ and c can be computed like

$$\xi = \frac{\hbar}{\sqrt{2mn_i \left| U_0 \right|}} \quad \text{and} \quad c = \sqrt{\frac{\left| U_0 \right| n_i}{2m}}, \quad (2)$$

where $U_0 = gN$. From now on all equations and computations will be limited to a 1D realm.

A. Time-independent solution for the bright soliton

Two soliton solutions can be found for equation 1, however this work will center on the bright soliton, which is the solution one can found for the case of an attractive interaction potential ($g < 0$). One shall begin by solving the time-independent equation, by substituting $i\hbar\partial_t\psi$ for $\mu\psi$, where μ is the condensate's chemical potential:

$$\mu\psi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial^2 x} + gN\left|\psi(x)\right|^2\psi(x). \tag{3}$$

Here, V has been taken to be zero. The bright soliton is known to have the form [7]

$$\psi = \psi_0\frac{1}{\cosh\left(\frac{x}{\sqrt{2}\xi}\right)}. \tag{4}$$

By substituting it onto equation 3, an equation involving ψ_0 and ξ is found, which reads:

$$\mu\psi = -\frac{\hbar^2}{4m\xi^2}\left[1 - 2\,\mathrm{sech}^2\left(\frac{x}{\sqrt{2}\xi}\right)\right]\psi + gN\left|\psi\right|^2\psi. \tag{5}$$

For this relation to hold, two conditions must be met for the constants on the solution,

$$\xi^2 = -\frac{\hbar^2}{2gNm\left|\psi_0\right|^2} \quad \text{and} \quad \mu = \frac{1}{2}gN\left|\psi_0\right|^2. \tag{6}$$

Note that ξ presents the same form as the expected, which was presented in equation 2.

III. GROSS-PITAEVSKII IN A HARMONIC OSCILLATOR

As seen in [7], one can subject a Bose Einstein Condensate to a harmonic potential with of the form

$$V(x) = \frac{1}{2}m\omega^2x^2, \tag{7}$$

which introduces a new set of variables into the equation:

$$a_0 = \sqrt{\frac{\hbar}{m\omega}} \quad \text{and} \quad \tau = \frac{1}{\omega}, \tag{8}$$

where a_0 represents the oscillator's distance units, and τ its time units. This is useful for obtaining a dimensionless GP equation by substituting $\tilde{x} = x/a_0$ and $\tilde{t} = t/\tau$ into equation 1:

$$i\hbar\frac{1}{\tau}\frac{\partial\tilde{\psi}}{\partial\tilde{t}} = -\frac{\hbar^2}{2m}\frac{1}{a_0^2}\frac{\partial^2\tilde{\psi}}{\partial\tilde{x}^2} + \frac{1}{2}m\omega^2\tilde{x}^2a_0^2\tilde{\psi} + gN\left|\tilde{\psi}\right|^2\tilde{\psi}, \tag{9}$$

which can be simplified to

$$i\frac{\partial\tilde{\psi}}{\partial\tilde{t}} = -\frac{1}{2}\frac{\partial^2\tilde{\psi}}{\partial^2\tilde{x}} + \frac{1}{2}\tilde{x}^2\tilde{\psi} + \tilde{g}N\left|\tilde{\psi}\right|^2\tilde{\psi}. \tag{10}$$

Here, the interaction constant is modified to $\tilde{g} = g/\hbar\omega$, which makes clear that this equation has $\hbar\omega$ defined as its energy units. In these new units, the relation between the interaction strength and the healing length reads

$$\tilde{U_0} = -\frac{1}{2\tilde{n_i}\tilde{\xi}^2}. \tag{11}$$

IV. NUMERICAL SOLVERS

Even though some specific cases of the Gross-Pitaevskii equation are already solved analytically, there are others, more complex, that must be solved numerically. Specifically, the experiments that will be carried out are only solvable that way. There are multiple ways one can numerically solve a parabolic differential equation such as the Schrodinger equation. For this work, the Crank Nicolson method was used [8]:

By discretizing both time and space dimensions, one can approximate their respective derivatives, and compute the time evolution via solving a simple matrix equation of the form $A_\beta^{j+1i}\psi_i^{j+1} = B_\beta^{ji}\psi_i^j$, where A is a tridiagonal matrix.

The behavior of the Crank Nicolson method, however is strongly affected by the value of the r parameter, computed as

$$r = K\cdot\frac{dt}{dx^2}, \tag{12}$$

where K is a multiplicative factor that depends on the equation being solved. This parameter needs to be smaller than around 0.5 for the solver to give reliable results, and for the entirety of this work, dx and dt were always set to ensure that r stayed at 0.3.

For the sake of this essay, a flexible and fast simulation software for Bose Einstein Condensates was needed, so BEC-Simulations was developed [9]. This tool allows the user to specify any starting wave function and potential for the condensate in a simple manner, and then simulates the dynamics of the system over time, giving the full evolution as an output. Other utilities were developed to analyze the results of the simulation, which can also be found in [9]. Furthermore, multiple tests were conducted to ensure the simulator works correctly, by checking the norm, energy and shape and form of the solutions without any external potential.

On top of that, to accelerate the simulation process, this program uses `JAX` instead of relying solely on `numpy` to perform calculations on the GPU, meaning that large system computations can be parallelized and run around 1.2 times faster on average (on an Nvidia RTX 3060 graphics card).

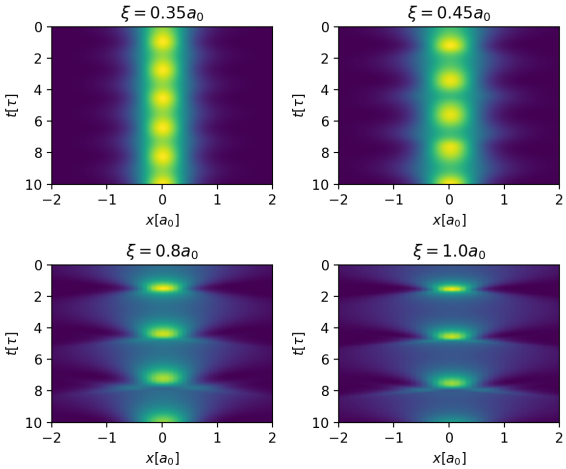

Figure 1. Density of the condensate as a function of time for four different values of the healing length: (a) $\xi = 0.35a_0$, (b) $\xi = 0.45a_0$, (c) $\xi = 0.8a_0$ and (d) $\xi = a_0$.

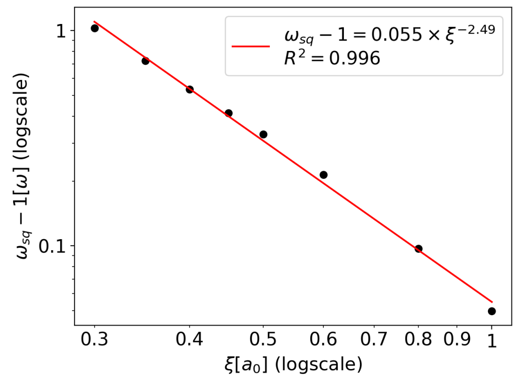

Figure 2. Dependency of the logarithm of the squeezing frequency of a soliton (ω_{sq}) with respect to the logarithm of its healing length (ξ), when placed in the center of a harmonic trap.

V. SIMULATION: SOLITON DYNAMICS IN A HARMONIC OSCILLATOR

When subjecting a soliton to a harmonic oscillator, one should expect the following two effects to happen: Any solution's expected position should follow a classical-like path, oscillating around the center at the frequency of the potential. In addition, if the solution is not a pure eigenstate of the potential (in fact, solitons are not), its form should change over time in a periodic manner. The latter effect is usually called "squeezing" or "breathing", and its frequency (ω_{sq}) should be a function of the relation between the healing length and the potential's width.

A. Squeezing soliton

A potential was set with the form $V = x^2/2$, and multiple solitons (with various healing lengths) were simulated, starting at the center of it. Figure 1 shows how every condensation studied presenter a breathing effect, but their frequencies varied, decreasing as the soliton got wider.

When plotting the squeezing frequency over the healing length, a very obvious relation arose: ω tended to 1 (the potential's frequency) as ξ got bigger, and approached infinity as ξ approached zero. This becomes obvious when fitting a line through a log-log diagram, as in figure 2.

In this figure, ω_{sq} is shown too follow a relation that reads

$$\omega_{sq} = 1 + 0.055 \times \xi^{-2.49}. \tag{13}$$

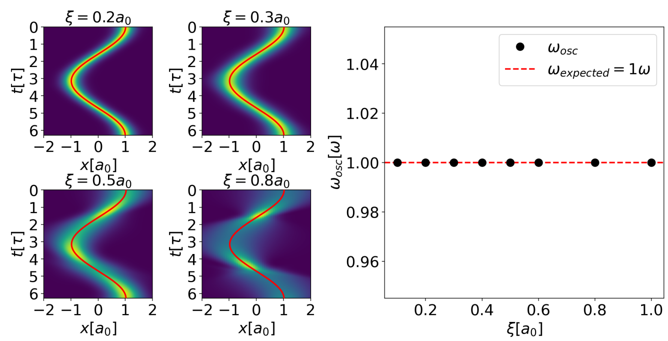

Figure 3. (a) Density of an oscillating soliton in a quantum harmonic oscillator as a function of time, with four different healing lengths: (a1) $\xi = 0.2a_0$, (a2) $\xi = 0.3a_0$, (a3) $\xi = 0.5a_0$ and (a4) $\xi = 0.8a_0$. (b) Oscillating frequency of a soliton placed in a quantum harmonic oscillator as a function of its healing length: the black dots correspond to the simulations, and the red dashed line to the potential's frequency.

B. Oscillating soliton

As a test of the numerical solver, multiple simulations of the Kohn mode of oscillation were computed. When studying the dynamics of a soliton displaced from the origin (at $x_0 = 1a_0$) in a harmonic oscillator, it should always follow the frequency of the oscillator. Different values of the soliton's healing length were used to cross-check this, as seen in figure 3, which all yielded the expected result.

VI. PHYSICS OF THE INVERTED HARMONIC POTENTIAL

If instead of a harmonic oscillator, one inverts the potential, one of two things should be expected to happen: If the potential has a length a_0 small enough compared to the soliton's width, it should break apart, or at least

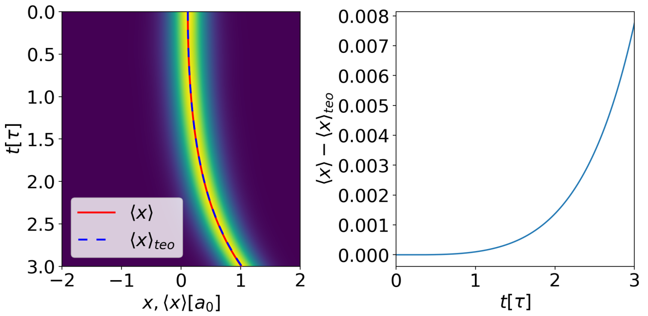

Figure 4. Density as a function of time of a soliton with healing length $\xi = 0.2a_0$ falling on the side an inverted harmonic potential. The red line on the left corresponds to the expectancy of the position of the soliton. The green line corresponds to the classical falling particle trajectory. The right plot shows the difference between the two as a function of time.

widen significantly; however, if the soliton has a strong enough interaction strength compared to the potential (its width is smaller than a_0), it should maintain its form and behave like a particle, falling, as such, entirely to one side of the potential.

An example of this can be seen on figure 4, which shows a relatively small soliton falling almost completely to one side of the potential. One can compare the expected value of its position to the classical particle falling off an inverted harmonic potential. Solving for $x(t)$,

$$\begin{aligned} V(x) &= -\frac{1}{2}x^2, \\ \ddot{x} = F &= -\nabla V(x) = x, \\ x(t) &= Ae^{-t} + Be^{t} \end{aligned} \tag{14}$$

and, finally, imposing that $x(0) = x_0$ and $\dot{x}(0) = 0$, a particular solution can be optained, which reads

$$x(t) = \frac{x_0}{2}(e^{-t} + e^{t}) = x_0 \cosh{(t)}. \tag{15}$$

The aforementioned figure shows a close resemblance between the classical and simulated evolution for the expected position of the soliton. However, when looking at the width of the solution (taken as the standard deviation of its position at each time), this should show a behavior that depends on the original healing length of the soliton.

To prove that, figure 5 shows the simulations of solitons with different healing lengths positioned on top of the potential. This figure seems to show a clear difference on the evolution of σ for small and large solitons. This dependency is further proven on image 6, where a clear transition is proven to arise around $\xi \approx 0.30 \pm 0.05a_0$. Below that, the condensation proved to stay put and unaltered over time. In contrast, above the transition point,

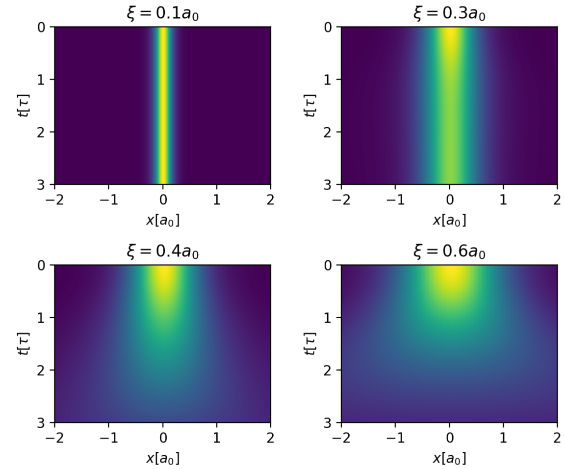

Figure 5. Density as a function of time of a soliton placed on top of an inverted harmonic oscillator, with four different healing lengths: (a) $\xi = 0.1a_0$, (b) $\xi = 0.3a_0$, (c) $\xi = 0.4a_0$ and (d) $\xi = 0.6a_0$.

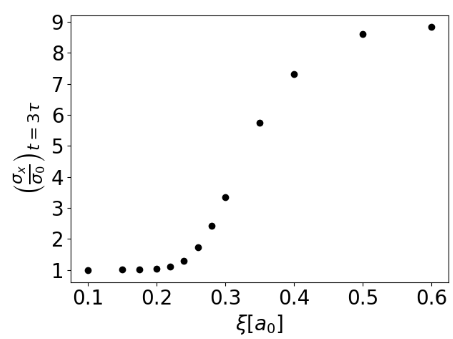

Figure 6. Dependency of the widening factor (standard deviation of the position at a fixed time $t = 3\tau$ over the initial standard deviation σ_0) of a soliton subjected to an inverted harmonic potential, depending on the starting healing length of the solution.

the condensation quickly broke apart upon starting the simulation.

An even more interesting result was found when combining the two above effects: One can repeat the latter experiment (Letting σ evolve with different starting ξ) but displacing the soliton $0.1a_0$ to the right. In this study case, results showed, a clear change in behavior: for small enough solitons, the full condensation fell to one side of the potential. However, when making the soliton big enough, it broke apart before starting to fall. This can be seen in figure 7

When plotting σ/σ_0 at a fixed time, with respect to the initial ξ (figure 8), a very similar result to the previous study was found, in fact, the same transition appeared ($\xi \approx 0.30 \pm 0.05a_0$).

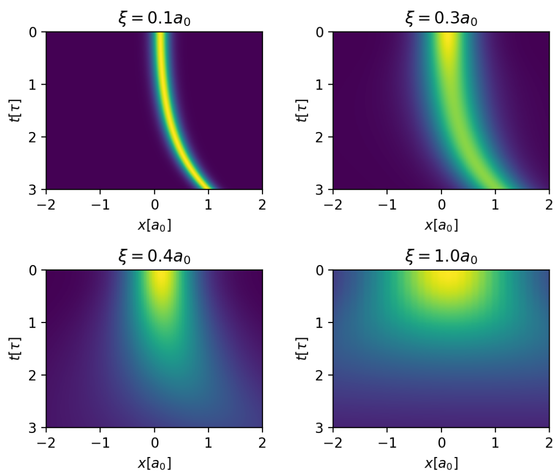

Figure 7. Density over time of a soliton placed slightly to the right ($x_0 = 0.1a_0$) of an inverted harmonic oscillator, with four different healing lengths: (a) $\xi = 0.1a_0$, (b) $\xi = 0.3a_0$, (c) $\xi = 0.4a_0$ and (d) $\xi = 1.0a_0$.

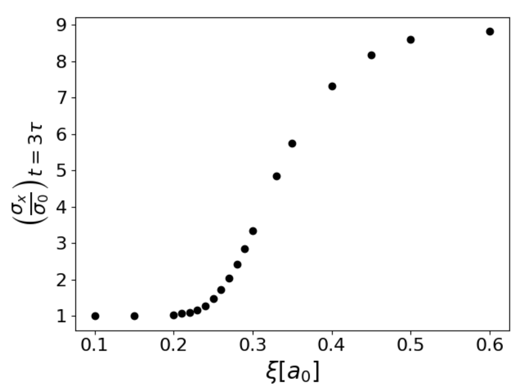

Figure 8. Dependency of the standard deviation of the position at a fixed time ($t = 3\tau$)of a soliton slightly displaced to the right of an inverted harmonic potential, depending on the starting healing length of the solution.

VII. CONCLUSIONS

In conclusion, this work has explored the dynamics of a Bose-Einstein Condensate, focusing on a soliton configuration within the condensate, by describing it via the Gross-Pitaevskii equation. The time-independent solution for the bright soliton was derived, and then, a harmonic oscillator term was incorporated into the equation, which resulted in a new set of units. These units allowed for a dimensionless form of the equation to be found, enabling numerical simulations using the Crank-Nicolson method.

Via a proprietary simulation software, the dynamics in a harmonic oscillator were explored, and two main vibration modalities arose: the Kohn oscillation mode, which showed the same frequency as the potential's, and the squeezing or breathing mode, the frequency of which manifested a dependency on the soliton's healing length of the form $\omega_{sq} = 1 + 0.055 \times \xi^{-2.49}$.

Finally, the dynamics in an inverted harmonic oscillator were also explored, proving that two scenarios occur for a soliton placed on top of it, which depended on its healing length. Wider solitons broke apart, whereas narrow solitons were more likely to keep their form and fall to a single side of the potential. A possible transition between these behaviors was observed around a healing length of $\xi \approx 0.30 \pm 0.05a_0$. On top of that, the expected position of the soliton was shown to closely resemble the classical trajectory.

Overall, this study on the dynamics of solitons in different potentials, provided valuable insights into their behavior and interaction with the potential. These findings enhanced our understanding of soliton physics and have potential applications in finding new ways to confine and control Bose-Einstein Condensations.

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