ASSIGNMENT 1

Exploring the Gross-Pitaevskii Equation: Theory and Simulation.

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Abstract

In our study, we delve into an analysis of a Bose-Einstein Condensate (BEC) subjected to a harmonic trap. By employing the Gross-Pitaevskii model, we simulate the system under various scenarios. Initially, we simulate it for the case of a null interaction potential, which reveals that $\bar{\mu}$ equates to the energy per particle for the harmonic oscillator. Subsequently, we simulate the Gross-Pitaevskii model for systems with different numbers of particles, observing that the kinetic energy diminishes as we increase the particle count. This observation leads us to the Thomas-Fermi approximation, which considers the kinetic term as negligible. To verify the validity of this approximation, we simulate the density profiles for a system of $N = 10^4$ and $N = 10^5$ bosons, finding that the Thomas-Fermi approximation replicates the results more accurately for the case of $N = 10^5$. Lastly, we derive the Virial theorem, establishing a relationship between kinetic energy, harmonic potential energy, and interaction energy, and setting the foundation for its verification through simulations.

1. Introduction

1.1. Gross-Pitaevskii equation.

The motivation for the Gross-Pitaevskii equation lies in obtaining the wave function that describes the lowest energy state of the many-body Hamiltonian:

$$H = \sum_{i=1}^{N} \left[\frac{\vec{p_i}^2}{2m} + V_{ext}(\vec{r_i}) \right] + \frac{1}{2} \sum_{i \neq j} V(r_{ij}) \tag{1}$$

Therefore, we employ the variational method to find an approximate many-body ground state wave function $|\psi\rangle$, leading to an upper bound for the ground state energy[1]:

$$E(\psi) = \frac{\langle \psi | \, H \, | \psi \rangle}{\langle \psi | \psi \rangle} \tag{2}$$

In our specific problem, the interactions are weak; hence, the influence of the entire system on a single boson is appropriately approximated by a mean field. We therefore use a normalized, symmetrized many-body wave function of the form:

$$|\psi\rangle = \big|\varphi(1)\varphi(2)\dots\varphi(N)\big\rangle \tag{3}$$

Applying the variational principle, our objective is to find the state φ that minimizes (2). Carrying out the calculation of (2) for the many-body Hamiltonian (1) we obtain:

$$E(\psi) = N \left\langle \psi \left| -\frac{\hbar^2 \nabla^2}{2m} + V_{\text{ext}}(\vec{r_i}) \right| \psi \right\rangle + \frac{N(N-1)}{2} (\varphi\varphi | V | \, \varphi\varphi) \tag{4}$$

To find the φ that gives us the minimum value, we will perform a functional derivative of the previous expression, enforcing that ψ is properly normalized using a Lagrange multiplier λ. As our expression contains both φ and φ^*, we can carry out the variational derivative with respect to either of the two functions. For convenience, we will perform the functional derivative with respect to the imaginary part, φ^*:

$$\frac{\delta}{\delta \varphi^*} \left[\langle \psi | \, H \, | \psi \rangle - \lambda \, \langle \psi | \psi \rangle \right] \tag{5}$$

Carrying out this calculation leads to the following equation, which must be solved iteratively: [2]

$$\left[-\frac{\hbar^2 \nabla^2}{2m} + V_{\text{ext}}(\vec{r}) + (N-1) \int d\vec{r} |\varphi(\vec{r})|^2 V(|\vec{r} - \vec{r'}|) \right] \varphi(\vec{r}) = \lambda \varphi(\vec{r}) \tag{6}$$

Our motivation centers on giving physical meaning to the Lagrange multiplier λ that we have introduced. This meaning is given by Koopman's theorem, which tells us that λ is simply the chemical potential of the system, μ [3].

To derive the Gross-Pitaevskii equation, we must make two approximations:

- Consider an effective potential of the form $V = g\delta(\vec{r'} - \vec{r})$ with $g = 4\pi\hbar^2 a_s/m$ the coupling constant and a_s the scattering length.
- Treat the limit of large N so that $N - 1 \simeq N$

With these considerations, we finally obtain the time-independent Gross-Pitaevskii equation:

$$\left[-\frac{\hbar^2 \nabla^2}{2m} + V_{\text{ext}}(\vec{r}) + gN|\varphi(\vec{r})|^2 \right] \varphi(\vec{r}) = \mu \varphi(\vec{r}) \tag{7}$$

1.2. Application of the Gross-Pitaevskii Equation for a Harmonic Trap.

The application of interest in our study pertains to the case of N identical bosons subjected to a mag-

netic field, represented by an external harmonic oscillator potential. In ultra-cold temperatures, close to absolute zero, these bosons form a Bose-Einstein condensate (BEC) composed of ^{87}Rb atoms. To evade recombination effects prevalent in ultra-cold gases, we operate under very low densities, thereby ensuring weak interactions among the bosons. Knowing that our potential is of the form $V_{\text{ext}}(\vec{r}) = \frac{1}{2}m\omega^2 r^2$, we can rewrite equation (7) in oscillator units, i.e., in units of $a_{ho} = \sqrt{\hbar/(m\omega)}$ and energies in units of $\hbar\omega$. This implies introducing $\vec{r}_{ho} = \vec{r}/a_{ho}$, $\bar{E} = E/(\hbar\omega)$, $\bar{\mu} = \frac{\mu}{\hbar\omega}$ and $\bar{\varphi}(\vec{r}_{ho}) = a_{ho}^{3/2}\varphi(\vec{r})$:

$$\begin{aligned}\bar{\mu}\bar{\varphi}(\vec{r}_{ho}) = &-\frac{\nabla^2}{2}\bar{\varphi}(\vec{r}_{ho})\frac{1}{2}r_{ho}^2\bar{\varphi}(\vec{r}_{ho}) \\ &+ 4\pi\bar{a}N|\bar{\varphi}(\vec{r}_{ho})|^2\bar{\varphi}(\vec{r}_{ho})\end{aligned} \tag{8}$$

Here we have defined $\bar{a} = a_s/a_{ho}$, where a_s is the scattering length of the s-wave function. [4]

2. Simple Harmonic oscillator case.

In this section, we will conduct an initial simulation of the Gross-Pitaevskii equation, considering that the interaction term is null. Hence, equation (8) will be:

$$\bar{\mu}\bar{\varphi}(\vec{r}_{ho}) = -\frac{\nabla^2}{2}\bar{\varphi}(\vec{r}_{ho}) + \frac{1}{2}r_{ho}^2\bar{\varphi}(\vec{r}_{ho}) \tag{9}$$

In this way, we have retrieved the Schrödinger equation for the standard harmonic oscillator. However, instead of the energy per particle, we have the chemical potential. In other words, we have an eigenvalue problem of the form $\mathcal{H}\bar{\varphi}(\vec{r}_{ho}) = \bar{\mu}\bar{\varphi}(\vec{r}_{ho})$. Consequently, we should find that the chemical potential corresponds to the single-particle energy of the Hamiltonian with a harmonic potential. Performing the calculation of this single-particle energy with the harmonic potential, we obtain [5]:

$$\begin{aligned}E_{n_1,n_2,n_3} =&\hbar\omega_1\left(n_1+\frac{1}{2}\right)+\hbar\omega_2\left(n_2+\frac{1}{2}\right) \\ &+\hbar\omega_3\left(n_3+\frac{1}{2}\right)\end{aligned} \tag{10}$$

Considering that the oscillator of the problem is isotropic $\omega_1 = \omega_2 = \omega_3$, working in energy units of the oscillator, and remembering that the energy we are calculating is the ground state energy, so $n_1 = n_2 = n_3 = 0$, through the simulation, we should obtain:

$$\bar{E} = \frac{3}{2} \tag{11}$$

Numerically calculating the solution to the Gross-Pitaevski equation without interaction potential and $N = 10^6$ bosons, we obtain $\bar{\mu} = 1,499967$, which agrees with the value $3/2$.

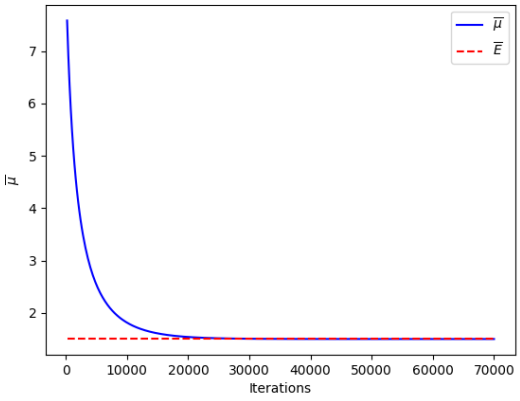

Figure 1: In this plot, it is shown how the chemical potential converges to the single-particle energy of our variational method, obtaining $\bar{\mu} = \bar{E} = \frac{3}{2}$.

3. Dependence on the number of particles

In this section, our focus is on solving the Gross-Pitaevskii equation using the same previously provided values. We aim to investigate how the chemical potential, total energy, kinetic energy, as well as the contributions from the harmonic and interaction terms, depend on the number of particles. Specifically, we explore the cases where $N = 100, 1000, 10000, 100000$ and 1000000.

N	$\bar{\mu}$	$\bar{\epsilon}$	$\bar{\epsilon}_{kin}$	$\bar{\epsilon}_{ho}$	$\bar{\epsilon}_{int}$
10^6	42.1190	30.1200	0.0612	18.0600	12.0000
10^5	16.8466	12.1039	0.1237	7.2376	4.7426
10^4	6.8659	5.0415	0.2404	2.9768	1.8243
10^3	3.0445	2.4247	0.4375	1.3674	0.6198
10^2	1.7874	1.6519	0.6561	0.8604	0.1355

Table 1: Numeric values of total energy per particle and its contributions (kinetic, interaction, harmonic oscillator) as well as the chemical potential as they evolve with the number of particles in the system.

Upon analyzing the Table 1, we observe that all energy contributions increase with the number of particles, except for the kinetic term. As the number of particles increases, the energy becomes more bound within the system, resulting in a decrease in the free movement of particles and a subsequent reduction in their kinetic energy. This trend aligns with the Thomas-Fermi approximation, which neglects the kinetic energy contribution and becomes more applicable at higher particle numbers.
The chemical potential measures the energy difference between a system with N particles and a system with $N-1$ particles. As we add particles to the system, extracting one becomes increasingly challenging due to the heightened interaction among the particles.
Furthermore, the interaction potential, which is of a contact-type $gN|\psi|^2$, naturally grows with the number of particles. The repulsive interaction combined with the harmonic oscillator trap leads to a decrease in density. Consequently, the probability of finding

particles at higher values of r_{ho} increases, resulting in higher harmonic potential energy.

4. Thomas-Fermi approximation.

Now we will proceed to perform the same study as in the previous section, but we will make use of the Thomas-Fermi approximation.

4.1. The Thomas-Fermi Limit.

The Thomas-Fermi limit is obtained by considering repulsive interactions such that $a > 0$ and is strong. In this way, the kinetic term can be neglected compared to the interaction and harmonic trap terms.

This results in equation (8) becoming: [4]

$$\bar{\mu}\bar{\varphi}(\vec{r}_{ho}) = \frac{1}{2}r_{ho}^2\bar{\varphi}(\vec{r}_{ho}) + 4\pi\bar{a}N|\varphi(\vec{r}_{ho})|^2\varphi(\vec{r}_{ho}) \qquad (12)$$

From this equation, knowing that $|\varphi(\vec{r}_{ho})|^2 = \rho(\vec{r}_{ho})$ and isolating it from the previous equation, we get:

$$\rho(\vec{r}_{ho}) = \frac{1}{4\pi\bar{a}N}\left(\bar{\mu} - \frac{1}{2}r_{ho}^2\right) \qquad (13)$$

Given this value, we can define the Thomas-Fermi radius r_{TF} as the radius at which the density becomes null, that is, where the parenthesis of the previous equation (13) becomes zero: $\bar{r}_{TF} = \sqrt{2\cdot\bar{\mu}}$. Therefore, imposing the normalization of density, we can obtain an expression for the chemical potential:

$$\int_0^{\bar{r}_{TF}} d\vec{r}\rho(\vec{r}_{ho}) = 1 \qquad (14)$$

By performing the calculation and isolating $\bar{\mu}$, we arrive at [4]:

$$\bar{\mu} = \frac{1}{2}(15N\bar{a})^{2/5} \qquad (15)$$

And by substituting this value for the expression of the Thomas-Fermi radius, we obtain:

$$\bar{r}_{TF} = (15\bar{a}N)^{1/5} \qquad (16)$$

4.2. Thomas-Fermi simulation.

We now attempt to study the same dependencies using the Thomas-Fermi approximation (12).
Setting the time derivatives to zero in our code (fred[i]=0 for all i), we get the following results [6]:

N	$\bar{\mu}$	$\bar{\epsilon}$	$\bar{\epsilon}_{ho}$	$\bar{\epsilon}_{int}$
10^6	42.0714	30.0520	18.0327	12.0194
10^5	16.9640	11.9640	7.1826	4.7814
10^4	6.6598	4.7634	2.8669	1.8964
10^3	2.6405	1.8984	1.1562	0.7421
10^2	1.0377	0.7647	0.4917	0.2730

Table 2: Numeric values of total energy per particle and its contributions (interaction, harmonic oscillator) as well as the chemical potential as they evolve with the number of particles in the system, using the Thomas-Fermi approximation ($\bar{\epsilon}_{kin} = 0$).

Just as we saw in Table 1, all energy contributions exhibit a consistent trend with an increase in the number of particles. It is worth noting that the kinetic energy term is omitted as it is inherently zero. A comparison between the combined harmonic potential and interaction energies demonstrates their alignment with the total energy $\bar{\epsilon}$.
We observe that, for smaller particle populations, the harmonic potential energy is lower compared to the GP result, while the interaction energy is relatively higher. This outcome is expected when neglecting the kinetic energy component. In such cases, the system becomes more confined, resulting in particles occupying lower values of r_{ho}. Consequently, the contribution from the harmonic oscillator is reduced due to its direct dependence on distance.

5. Density profile

We will plot the density dependence on the distance for $N = 1000$ and $N = 100000$, and compare the Gross-Pitaevski solution with the Thomas-Fermi approximation solution.

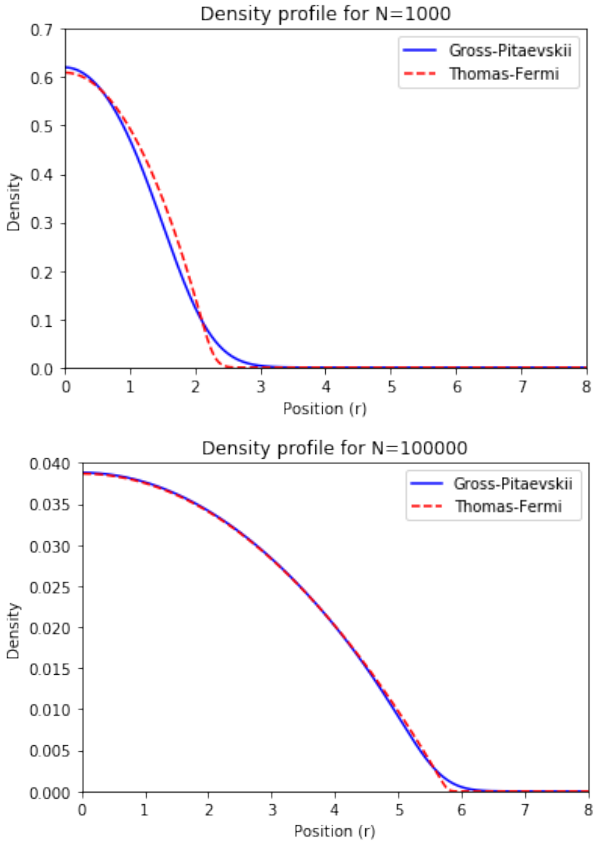

Figure 2: Density profiles for $N = 1000$ and $N = 100000$ particles with respect to the spatial position r.

In observing the Gross Pitaevski and Thomas-Fermi densities, we note that they closely mirror each other when $N = 10^5$. However, a slight difference is discernible at $N = 10^3$. As we touched upon earlier, the influence of the kinetic component tends to decrease as the quantity of bosons in the system escalates, while the interaction term assumes greater significance. Hence, as the particle system grows, the

Thomas-Fermi approximation aligns more accurately with the precise results.

6. Virial theorem

In this section, we will proceed to derive an expression that connects the kinetic energy E_{kin}, the energy of the harmonic potential E_{ho}, and the interaction energy E_{int}. In other words, we are going to deduce the expression of the Virial Theorem for this type of problems. Subsequently, we will analyze its verification through a simulation.

6.1. Expression of the Virial Theorem

Starting from the time-independent Gross-Pitaevskii equation in units of the harmonic oscillator (8), we can obtain an expression for the energy per particle in the following form: [4]

$$\frac{\bar{E}}{N} = \int d\vec{r_1} \left[\frac{|\nabla\bar{\varphi}(\vec{r}_{ho})|^2}{2} + \frac{1}{2} r_{ho}^2 |\bar{\varphi}(\vec{r}_{ho})|^2 + 2\pi\bar{a}N|\bar{\varphi}(\vec{r}_{ho})|^4 \right] \tag{17}$$

This can be broken down into the following contributions:

$$\begin{aligned} \bar{E}_{kin} &= N \int d\vec{r}_{ho} \frac{|\nabla\bar{\varphi}(\vec{r}_{ho})|^2}{2} \\ \bar{E}_{ho} &= N \int d\vec{r}_{ho} \frac{1}{2} r_{ho}^2 |\bar{\varphi}(\vec{r}_{ho})|^2 \\ \bar{E}_{int} &= N \int d\vec{r}_{ho} 2\pi\bar{a}N\bar{\varphi}(\vec{r}_{ho})|^4 \end{aligned} \tag{18}$$

Recalculating the energy per particle with this rescaled wave function, we find that:

$$\bar{\epsilon}(\lambda) = \lambda^2 \bar{\epsilon}_{kin} + \frac{1}{2}\bar{\epsilon}_{ho} + \lambda^3 \bar{\epsilon}_{int} \tag{19}$$

Deriving this expression with respect to λ and knowing that the minimum corresponds to $\lambda = 1$, we finally obtain the Virial relation:

$$\left.\frac{d\bar{\epsilon}}{d\lambda}\right|_{\lambda=1} = 0 = 2\bar{\epsilon}_{kin} - 2\bar{\epsilon}_{ho} + 3\bar{\epsilon}_{int} \tag{20}$$

6.2. Simulation of the Virial Theorem

We will now proceed to verify this result via simulation. Subsequently, we will plot $2\bar{\epsilon}_{kin} - 2\bar{\epsilon}_{ho} + 3\bar{\epsilon}_{int}$ for different values of N. Specifically, we will carry out the simulation for $N = 10^2$, 10^3, 10^4, 10^5, and 10^6. To observe the convergence of these results, we will plot the values of the expression (20) as a function of the number of iterations performed. In this way, we will be able to observe how the result converges to 0 as the number of iterations increases, thus verifying the Virial theorem.

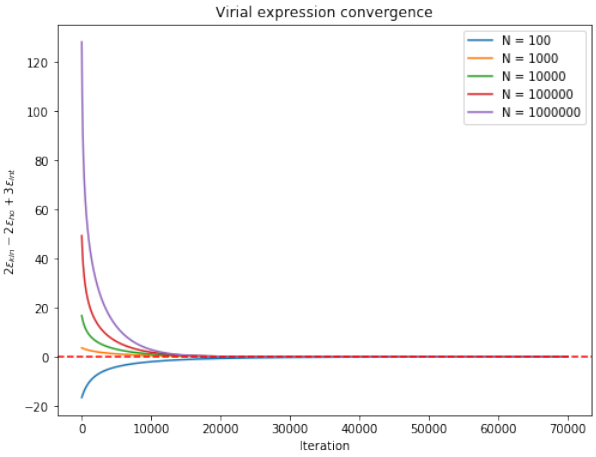

Figure 3: In this plot, it is shown how the expression for the Virial theorem apidly converges to zero with very few iterations, just as we expected.

7. Conclusion

In conclusion, this study has deepened our understanding of Bose-Einstein Condensates (BECs) within a harmonic trap, and the application and interpretation of the Gross-Pitaevskii equation. Utilizing code simulations (as referenced in [6]), we discerned a trend across systems with varying particle counts: as the particle number grows, there is a decrease in kinetic energy and increase in interaction energy. This behavior leads to a larger chemical potential, indicative of a more tightly bound system, and implying an increased difficulty in removing particles.

By comparing the Gross-Pitaevskii and Thomas-Fermi approximations, weobserve a trend of decreasing kinetic energy and increasing interaction energy with the growth of particle count, which lends credence to the applicability of the Thomas-Fermi approximation for larger systems. Moreover, through density profile comparisons, our study confirms the close alignment of the Gross-Pitaevskii and Thomas-Fermi models in high particle-count systems.

In addition, we have deduced an expression of the Virial theorem that ties together kinetic, harmonic potential, and interaction energies, a connection we have been able to confirm through simulation.

Collectively, these findings give us a more nuanced understanding of BECs through the lens of the Gross-Pitaevskii equation, illuminating the regime in which the Thomas-Fermi approximation delivers accurate descriptions.

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