Mecànica quàntica de N-cossos i sistemes ultrafreds

Weakly interacting and confined bosons at low density

P. Fargas Reixats; A. Fernández García

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To solve this problem we have written a new code in Python, based on the Fortran code that was given to us along with this task.

The code can be found in *pfargas/Grosspitaevskii*. The code is thought to be easy for an end user to use through a notebook.

This task has been done as a joint effort of the two authors: Pau Fargas developed and wrote the code in Python used to compute the solutions asked in this task, and Adam Fernández took care of the theory behind this problem and the redaction of this document. Despite that, both of us have understood and seen all parts of this work, from the software and coding part to the more theoretical one. The results obtained have been mutually discussed.

Gross-Pitaevskii equation in harmonic oscillator units: The time-independent Gross-Pitaevskii equation (GP) reads as follows:

$$\mu\varphi(\vec{r}) = -\frac{\hbar^2\nabla^2}{2m}\varphi(\vec{r}) + V_{ext}\varphi(\vec{r}) + gN|\varphi(\vec{r})|^2\varphi(\vec{r}) \ .$$

Where μ is the chemical potential, g a coupling constant, N the number of particles, $\hbar$ the reduced Planck constant, m the mass of the bosons, V_{ext} an external potential that acts like a trap and *varphi* the mono-particular wave function.

In the case of the GP equation in a harmonic potential, $V_{ext} = (1/2)m\omega^2 r^2$, it is useful to write it in terms of the oscillator units, namely, writing the distances in $a_{ho} = \sqrt{\hbar/(m\omega)}$ units, and the energies in $\hbar\omega$ units. Introducing $\vec{r}_1 = \vec{r}/a_{ho}$, $\bar{\mu} = \mu/(\hbar\omega)$ and $\bar{\varphi}(\vec{r}_1) = a_{ho}^{3/2}\varphi(\vec{r})$, and using that $g = 4\pi\hbar^2 a_s/m$ and $\bar{a}_s = a_s/a_{ho}$, we obtain the GP equation in harmonic oscillator:

$$\bar{\mu}\bar{\varphi}(\vec{r}_1) = -\frac{\nabla_1^2}{2}\bar{\varphi}(\vec{r}_1) + \frac{1}{2}r_1^2\bar{\varphi}(\vec{r}_1) + 4\pi\bar{a}_s N|\bar{\varphi}(\vec{r}_1)|^2\bar{\varphi}(\vec{r}_1) \ . \tag{1}$$

Notice that after this variable change the wave function is still normalized to 1:

$$\int d\vec{r}_1|\bar{\varphi}(\vec{r}_1)|^2 = \int d\vec{r}a_{ho}^{-3}|\varphi(\vec{r})|^2 a_{ho}^3 = 1 \ .$$

Imaginary time evolution To solve the time-independent GP equation, it will be used the imaginary time method.

The use of this method is motivated by its ability to transform an oscillating problem, such as the time evolution of the Schrödinger equation, into a diffusion one. Converting this evolution into a diffusion problem assures the convergence of the problem into the ground state for great times ($\tau \to \infty$).

This will start with the time-dependent GP equation:

$$i\hbar\frac{\partial}{\partial t}\bar{\varphi}(\vec{r}_1) = -\frac{\nabla_1^2}{2}\bar{\varphi}(\vec{r}_1) + \frac{1}{2}r_1^2\bar{\varphi}(\vec{r}_1) + 4\pi\bar{a}_s N|\bar{\varphi}(\vec{r}_1)|^2\bar{\varphi}(\vec{r}_1) \ . \tag{2}$$

This equation can be written as $\frac{\partial}{\partial t}\bar{\varphi}(\vec{r}_1) = -i\frac{\hat{H}}{\hbar}\bar{\varphi}(\vec{r}_1)$.

Then, if $\hat{H} \neq \hat{H}(t)$ the time-evolution operator is written as $U(t) = \exp\left(-\frac{i\hat{H}t}{\hbar}\right)$. Then, if we apply $\tau = it$, the time-dependant GP equation is:

$$\frac{\partial}{\partial\tau}\bar{\varphi}(\vec{r}_1) = -\frac{\hat{H}}{\hbar}\bar{\varphi}(\vec{r}_1) \ . \tag{3}$$

And the time-evolution operator then $U(\tau) = \exp\left(-\frac{\hat{H}\tau}{\hbar}\right)$.

To evolve the equation, it is needed an initial wave function or *ansatz*, which in our case it takes the form: $\psi_0(x, \tau = 0) = 2 \cdot \frac{\sqrt{\sigma^3}}{\sqrt{\sqrt{\pi}}} \cdot x \cdot \exp(-0.5 \cdot \sigma^2 \cdot x^2)$.

Which, in general, it can be written as $\psi(x, t = 0) = \sum_n c_n \varphi_n(x)$ where $\varphi_n(x)$ is the nth eigenstate.

The time evolution will proceed as follows:

$$\psi(x, \tau + \Delta\tau) = \psi(x, \tau) \exp\left(-\frac{\hat{H}\Delta\tau}{\hbar}\right) = \sum_n c_n \varphi_n(x) \exp\left(-\frac{E_n \Delta\tau}{\hbar}\right) ,$$

where E_n is the eigenvalue of the nth eigenstate.

If we let the state evolve, such that $\tau = \lim_{n\to\infty} n\Delta\tau$, thanks to the exponential decay of the diffusion problem, the only surviving term will be the one with the lowest energy, the ground state.

If we make $\Delta\tau$ small enough, the diffusion operator can be developed in Taylor's series, so the evolution can be written as:

$$\psi(x, \tau + \Delta\tau) = \psi(x, \tau) - \frac{\Delta\tau\mu(x)}{\hbar}\psi(x, \tau) \ . \tag{4}$$

This will be the equation used to evolve from ψ_0 to the ground state.

a0) The Schrödinger equation for an harmonic oscillator is

$$E\varphi(\vec{r}) = -\frac{\hbar^2\nabla^2}{2m}\varphi(\vec{r}) + \frac{1}{2}m\omega^2 r^2 \varphi(\vec{r}) \ .$$

In harmonic oscillator units (same variable change as in the GP case) is written as:

$$e\bar{\varphi}(\vec{r}_1) = -\frac{\nabla_1^2}{2}\bar{\varphi}(\vec{r}_1) + \frac{1}{2}r_1^2\bar{\varphi}(\vec{r}_1) \ , \tag{5}$$

where

$$e = \left(\frac{3}{2} + n_x + n_y + n_z\right) \ , \tag{6}$$

is the energy per particle.

If we set the interaction equal to zero, $\bar{a}_s = 0$, the Gross Pitaevskii equation becomes the Schrödinger equation in harmonic oscillator units (see equations 1,5). Therefore, μ becomes the eigenvalue of the Hamiltonian of a harmonic quantum oscillator, namely, its energy 6. Thus, if we use the code mentioned above to evolve the equation and obtain the values of the chemical potential μ as well as the energy per particle e in the ground state, these two values should be equal to 3/2. Indeed, for a number of particles $N = 1000000$, we obtain:

$$e = 1.50 \ , \qquad \mu = 1.50 \ .$$

This calculation can serve as an initial test to verify the correct behaviour of the code.

a) If we take $\bar{a}_s = 0.00433$, the scattering length of the ^{87}Rb, and we use the code we have written to solve the Gross-Pitaevskii equation for different numbers of particles, we obtain the results in Table 1.

N	μ	e_{kin}	e_{trap}	e_{int}	e
100	1.79	0.65	0.87	0.13	1.65
1000	3.04	0.44	1.37	0.62	2.42
10000	6.87	0.24	2.98	1.82	5.04
100000	16.85	0.12	7.24	4.74	12.10
1000000	42.12	0.06	18.05	12.00	30.12

Table 1: Table with the results obtained in the answer of question **a)**.

We can see that all the magnitudes studied increase with the number of particles in the system, except the kinetic energy per particle, which decreases. Therefore, the Thomas-Fermi approximation (TF) will be better the greater the number of particles.

b) The *Thomas-Fermi approximation* (TF) consists of supposing that the potential term $\hat{U} \equiv \hat{V}_{ext} + \hat{I}$ is much greater than the kinetic $\hat{T}$: $\hat{T} << \hat{U}$. This approximation allows us to neglect the kinetic term.

To solve the equation GP equation in the Thomas-Fermi approximation, we can not completely neglect the kinetic term, since we need its derivatives in order to evolve the system in the imaginary time method, as we have been doing. Nonetheless, we can make this term negligible in front of the other ones by multiplying it by a parameter.

In the code, the kinetic term is written as $\hat{T} = -\alpha\nabla^2$, where α is a variable we called `kinetic_coeficient`. In the general GP case, the `kinetic_coeficient` is set to 0.5 by instantiating an object with the `thomas_fermi` attribute to `False` (default value). To obtain the TF approximation in the code we just need to instantiate an object with the `thomas_fermi` attribute to `True`. This sets the variable `kinetic_coeficient` to 0.000000000000001, thus making this term negligible in front of the other ones.

By doing so, we obtain the following results.

N	μ	e_{kin}	e_{trap}	e_{int}	e
100	1.04	0.00	0.47	0.29	0.76
1000	2.65	0.00	1.15	0.75	1.90
10000	6.66	0.00	2.86	1.90	4.76
100000	16.75	0.00	7.18	4.78	11.96
1000000	42.08	0.00	18.03	12.03	30.05

Table 2: Table with the results obtained in the answer of question **b)**.

We see that the results obtained have the same behavior as the ones obtained in the previous section, but now the kinetic energy $e_{kin} \simeq 0$.

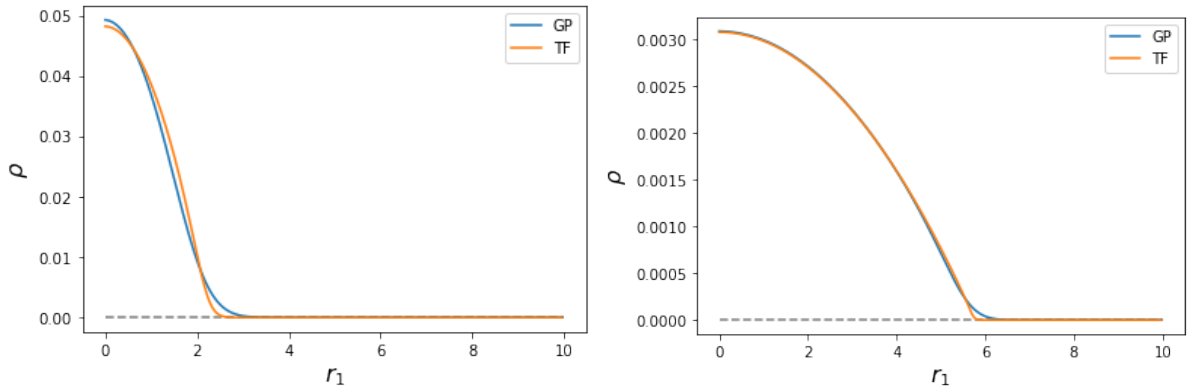
c) If we make a plot of the density profile $\rho(r_1)$ normalized such that

$$\int dr_1 r_1^2 \rho(r_1) = 1$$

for $N = 1000$ and $N = 100000$ particles, and compare both the GP and the TF results, we obtain the following figures (see 1a, 1b).

Both axes are in the harmonic oscillator units.

We observe that in the plot 1b, with $N = 100000$, the TF approximation fits better the general GP density, while in the plot 1a, for a smaller number of particles $N = 1000$, it does not. This is because, as we said in section **b)**, the kinetic energy e_{kin} decreases as the number of particles N increases, thus making the TF a better approximation for greater numbers of particles.



(a) N=1000 (b) N=100000

Figure 1: Plot of the density profiles for $N = 1000$ and $N = 100000$ for the GP equation and the TF approximation.

d) The Virial theorem for the Gross-Pitaevskii equation is obtained by scaling its solution as

$$\bar{\varphi}(\vec{r}) = \lambda^{3/2}\varphi(\lambda\vec{r}) \ .$$

This new wave function is also normalized to 1. Computing now the contributions to the trap, kinetic and interaction energy per particle with this new scaled wave function, we obtain:

$$e_{trap}(\lambda) = \frac{1}{\lambda^2}e_{trap} \ , \qquad e_{kin}(\lambda) = \lambda^2 e_{kin} \ , \qquad e_{int}(\lambda) = \lambda^3 e_{int} \ ,$$

such that

$$e(\lambda) = \frac{1}{\lambda^2}e_{trap} + \lambda^2 e_{kin} + \lambda^3 e_{int} \ .$$

The ground state of a system always has the minimum energy possible. Thus, in this state, $e(\lambda)$ has to be a minimum. If we minimize this function we obtain

$$\frac{de(\lambda)}{d\lambda} = \frac{-2}{\lambda^3}e_{trap} + 2\lambda e_{kin} + 3\lambda^2 e_{int} \ . \tag{7}$$

We know this is true for the original solution of the GP equation,
$Bar\varphi(\vec{r})$. Thus, for $\lambda = 1$ we recover this solution, and therefore the minimum condition 7 will be

$$\left.\frac{de(\lambda)}{d\lambda}\right|_{\lambda=1} = -2e_{trap} + 2e_{kin} + 3e_{int} \ .$$

This expression is the Virial theorem for the GP equation, and the solutions we found of the GP should fulfil it.

Indeed, if we check it numerically with the code we have written, for different values of N, we find that all the values obtained are close to zero. Thus, we can say that the Virial theorem is fulfilled.

N	1000000	100000	10000	1000
$2e_{kin} + 3e_{int} - 2e_{trap}$	0.025	0.00048	-0.0011	-0.012

Table 3: Table with the number of particles in the system and the Virial value calculated numerically

Note that this is a numerical resolution, and therefore, we will never obtain an exact 0. This is due to the limited numerical precision in computing and the resulting error it entails. Nonetheless, the values we have obtained are small enough to say that the Virial theorem is fulfilled.