Stability in Bose-Einstein Condensates

Author: Raquel Esteban Puyuelo.
Facultat de Física, Universitat de Barcelona, Diagonal 645, 08028 Barcelona, Spain.[*]
(Dated: June 16th 2014)

Abstract: In this work the validity of an analytic approximation expression [1] for the critical number of atoms that a Bose-Einstein Condensate can hold before collapsing when the interaction between them is attractive is checked. In order to do this the system is treated in a more precise way by numerically solving the Gross-Pitaevskii equation. One finds that the variational approach underestimates the number of atoms that can fit in a Bose-Einstein Condensate before it collapses.

I. INTRODUCTION

Bose-Einstein Condensation is among the most fascinating phenomena in nature as its surprising properties are direct consequences of quantum mechanics. In essence, it is a macroscopic quantum phenomena. Unlike the classical ideal gas or the Fermi-Dirac gas, the Bose-Einstein ideal gas has a thermodynamic phase transition which is driven by the particle statistics and not by their interaction. A Bose-Einstein Condensate (BEC from now on) is a state of matter of a dilute gas of cold atoms obeying Bose-Einstein statistics below a certain critical temperature (T_c), which is often called *condensation temperature* in analogy with the liquid-gas transition. This transition occurs when the de Broglie wavelength of the characteristic thermal motions becomes comparable to the mean interparticle separation. When this condition is attained, a macroscopic fraction of the bosons occupy the lowest single particle quantum state, even if the temperature is high enough to populate other states.

This omnipresent phenomenon plays remarkable roles in atomic, nuclear, elementary particle and condensed matter physics, as well as in astrophysics [2]. The study of BEC in weakly interacting systems has at its heart the possibility of revealing new macroscopic quantum phenomena that can be understood from first principles, and may also help advance our comprehension of superfluidity and superconductivity.

BEC was predicted by Bose (1924) and Einstein (1924, 1925) but eluded direct and unquestioning observation until 1995 as the experimental techniques for trapping and cooling atoms in magnetic and laser traps had been improved. The time-of-flight measures carried on these experiments on gases of rubidium [3] and sodium [4] showed a clear signature of the BEC: when the confining trap was switched off and the atoms were left to expand, a sharp peak in the velocity distribution below a certain critical temperature appeared.

Not all bosons can form condensates. For example, Helium, which is among the most famous bosons in Physics can not form BEC when it is in its ground state. This is because it is liquid at T=0 K and therefore correlations can not be neglected. On the other side, there are other atoms such as alkali that can be in this state of matter.

A. The stability problem

All BEC are essentially metastable gases that lack of cohesion and therefore it is compulsory to use a trap to confine them. Most of the times, the confining traps are well approximated by harmonic potentials of frequencies ω_x, ω_y, ω_z. Playing with these trap frequencies different shapes of the condensate can be achieved. For $\omega_x = \omega_y = \omega_z$ the cloud will be spherical, while axially symmetric geometries such as the so called cigar shape and disk/pancake shape can also be created both numerically and experimentally. A characteristic length scale for the systems can be defined: $a_{ho} = [\hbar/(m\omega_{ho})]^{1/2}$, where $\omega_{ho} = (\omega_x\omega_y\omega_z)^{1/3}$ is the geometric mean of the harmonic frequencies, m is the mass of the atoms in the gas and $\hbar$ is the reduced Plank constant.

Interactions between atoms can be either attractive or repulsive. While a trapped repulsive interacting BEC will always be stable, it is different if the interactions are attractive because that can imply instability to collapse if the number of atoms in the condensate is large enough. That shows that attractive interacting condensates can exist, but only up to a critical number of atoms N_{cr}. Thus, there are stability conditions for a small number of atoms such as lithium-7 [5] in trapped condensates. In these cases, the zero-point kinetic energy provided by the trap can balance the increase of the center density due to the attraction of the atoms for each other. It should be noted that cigar and pancake geometries are obviously less stable than the spherical one if atoms interact attractively because less atoms can fit in one of the directions of the trap and the critical number N_{cr} is thus reached sooner. Stability conditions in this last two geometries are analytically more difficult to consider, only the spherical geometry will be studied here because the aim of this work is to check the approximate expression given in [1], which treats only spherical symmetries.

There are different experimental ways in which a BEC can be produced, but they all share two common features: cooling down to the temperatures (between μK and nK) at which the condensates take place and trapping [6]. These techniques are laser cooling and magneto-optical

*Electronic address: restebpu8@alumnes.ub.edu

trapping, which combines Doppler cooling and magnetic trapping. This laser based-methods were developed in the 1980s and were the key to the first observations of this phenomenon.

II. THEORY

A. Gross-Pitaevskii equation deduction

Although in the standard literature the Gross-Pitaevskii equation is usually obtained in the framework of the second quantisation formalism, it is possible to motivate the derivation of the GPE in relationship to concepts from statistical physics.

As it was discussed above, a BEC is obtained from a collection of N bosons in their ground state at very low temperatures. The general N-body Hamiltonian for identical particles of mass m can be expressed as follows

$$\hat{H} = \sum_{i=1}^{N} \left[-\frac{\hbar^2}{2m}\nabla_i^2 + V_{ext}(\vec{r}_i) \right] + \frac{1}{2}\sum_{i=1}^{N}\sum_{i\neq j}^{N} V(|\vec{r}_i - \vec{r}_j|), \tag{1}$$

where the first term in the Laplacian is the kinetic energy, V_{ext} represents the external trapping potential and V represents the pair interaction between the N particles.

The ground state of the system corresponds to the minimum energy, which can be found approximately by minimizing the expectation value of (1) using a totally symmetric trial wave function that is the product of single particle states:

$$|\Psi(1, 2, ..., N)\rangle = |\varphi(1)\rangle \otimes |\varphi(2)\rangle \otimes ... \otimes |\varphi(N)\rangle . \tag{2}$$

This *ansatz* can be made as in the dilute situation one can expect that correlations are negligible. Furthermore, the bosons interact weakly, so that a mean field approximation can be used, which means that the action felt by a given particle due to the rest is substituted by the average effect of the interactions of this particle and the $(N-1)$ other particles.

Following a similar deduction to the Hartree-Fock equations for fermions that can be found in standard textbooks [7], the GPE can be obtained. The total energy $\langle\Psi| H |\Psi\rangle$ will be minimized together with the constraint of normalization $\langle\Psi|\Psi\rangle = N$, so $|\Psi|^2$ represents the number of particles:

$$\delta[\langle\Psi| H |\Psi\rangle - \lambda \langle\Psi|\Psi\rangle] = 0. \tag{3}$$

It can be proved that the Lagrange multiplier λ used in the minimization can be identified with the chemical potential μ of the system (the energy required to add one more atom to the condensate), which what the Koopman's theorem [7] states. That leads to the following equation:

$$-\frac{\hbar}{2m}\nabla^2\varphi(\vec{r}) + V_{ext}\varphi(\vec{r}) + (N-1) \times \left[\int d\vec{r'} V(|\vec{r}-\vec{r'}|)|\varphi(\vec{r})|^2\right]\varphi(\vec{r}) = \mu\varphi(\vec{r}). \tag{4}$$

As condensate atoms interact by means of binary collisions, at low temperatures only s-wave collisions are important. Assuming that the gas is dilute and weakly interacting, the interaction between particles can be written in term of the scattering length using a zero-range interaction potential such that

$$V(|\vec{r}-\vec{r'}|) = g\delta(\vec{r}-\vec{r'}) = \frac{4\pi\hbar^2}{m}a_s\delta(\vec{r}-\vec{r'}), \tag{5}$$

where g is the coupling constant and a_s is the s-wave scattering length, which measures the interactions between the bosons and can be attractive ($a_s < 0$) or repulsive ($a_s > 0$). It is worth noting that this quantity is nowadays tuneable by means of Feshbach ressonances [8].

For a large enough number of atoms, one can use the approximation that $N-1 \approx N$, which leads to the Gross-Pitaevskii equation (GPE):

$$-\frac{\hbar^2}{2m}\nabla^2\varphi(\vec{r}) + V_{ext}(\vec{r})\varphi(\vec{r}) + g|\varphi(\vec{r})|^2\varphi(\vec{r}) = \mu\varphi, \tag{6}$$

where all the atoms are assumed to be in the condensate at T =0 K. This equation considers that the system is at zero temperature, which works fine for BEC as the temperatures at which they take place are very low and close to the absolute zero. Furthermore, when the gas is very dilute and weakly interacting (na_s^3 <<1), where n is the average density, considering that all the atoms are in the condensate fraction is very accurate. For example, more than 99% of the alkali atoms are in the condensate at $T = 0$ K.

Solving this nonlinear equation for the wave function must be done numerically but nonetheless it shows a form of BEC: the population of the lowest state in energy becomes macroscopic under the right conditions.

B. Stability deduction (collapse for attractive forces)

If the trapped gas has attractive interactions ($a_s < 0$) its central density will increase when new particles are added to the cloud. This happens in order to lower the particle interaction density, which can be stabilized by the zero-point kinetic energy. However, if the central density increases too much, this kinetic energy is no longer able to avoid the collapse of the gas. For a given atomic species, the collapse is expected to occur when the number of condensed particles exceed a critical value N_{cr}.

In the literature [1] there is an expression that explains the behavior of the trapped gas with attractive forces at T =0 K. It allows oneself to obtain the critical number N_{cr} of bosons that a BEC can hold before it collapses. It does it by means of a variational method that uses a Gaussian as a trial wave function [9] due to its similarity to the experimental density and for the sake of obtaining a simple expression.

A spherical trap can be described by this *ansatz*, which is expressed in oscillator length a_{ho} units:

$$\varphi(r) = \left(\frac{N}{w^3 a_{ho}^3 \pi^{3/2}}\right)^{1/2} \exp\left(-\frac{r^2}{2w^2 a_{ho}^2}\right), \quad (7)$$

where w is a dimensionless parameter which fixes the width of the Gaussian (condensate).

The energy functional that describes the system

$$E[\varphi] = \int d\vec{r} \left[\frac{\hbar}{2m}|\nabla\varphi|^2 + V_{ext}(\vec{r})|\varphi|^2 + \frac{g}{2}|\varphi|^4\right], \quad (8)$$

is minimized giving as a result the energy per particle in oscillator units:

$$\frac{E(w)}{N\hbar\omega_{ho}} = \frac{3}{4}(w^{-2} + w^2) - (2\pi)^{-1/2}\frac{N|a|}{a_{ho}}w^{-3}. \quad (9)$$

Numerical calculation of the critical value $w_c = w_{cr}$ can be performed. As these value is reached when the function (9) has an inflection point, it must be required that its first and the second derivative vanish at the critical point. By doing this one founds $w_{cr} \approx 0.6689$ and combining this value with equation (9) it can be found the relationship between the critical number of atoms that can be in the condensate and the adimensional ratio between the s-scattering length and the oscillator characteristic length:

$$N_{cr}|a_s|/a_{ho} \approx 0.6706. \quad (10)$$

This is plotted in Figure 1, which shows the energy per particle in oscillator units that is obtained from the variational method described above as a function of the effective Gaussian cloud width w. Several curves for different values of $N|a_s|/a_{ho}$ are shown in order to reflect the behavior before and after the collapse. It can be seen that the local minimum disappears at $N = N_{cr}$, value for which the collapse happens. From (10) an estimation of the critical number of particles in a condensate given a_s and a_{ho} can be obtained.

C. Numerical calculation of the GPE

As the nonlinear equation (6) can not be solved analytically, a numerical code must be used in order to check the validity of the variational result (9). This code solves numerically the three dimensional GPE and provides the energy of the fundamental state of the BEC. It is based in a space discretization in a grid of 72×72×72 points with a separation of 0.5 Å, which means that the wave functions will also be discretized on a three dimensional spatial mesh. All the derivatives in the code are calculated using 13-point centered formulas in order to have the maximum accuracy in the results.

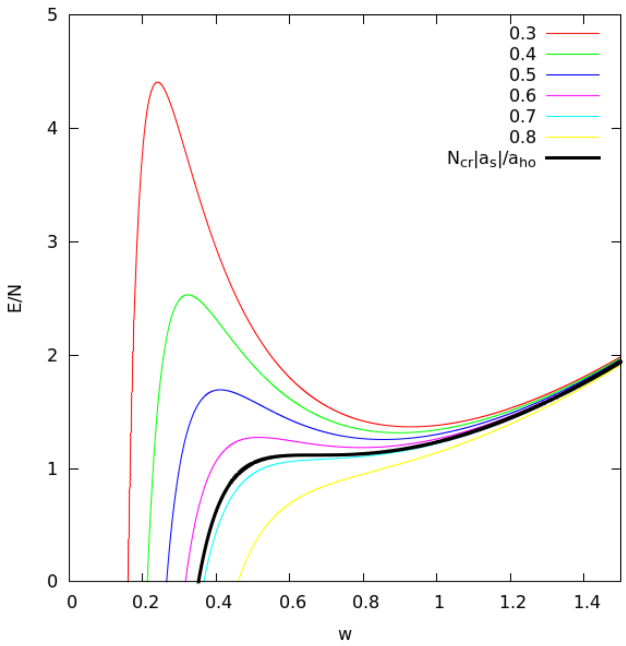

Figure 1: Energy per particle in oscillator units ($\hbar\omega_{ho}$) obtained from the variational calculation for an attractive condensate in an spherical trap is plotted versus the adimensional width of the Gaussian function w. The black thick line corresponds to N_{cr}.

To compute the solution the code follows an iterative numerical method based on the *Imaginary step time method* [10]. To start the calculation, an initial guess value must be provided; in this case, in order to avoid any kind of bias a random function is used. In addition, as the code relies on iterative procedures, the process finishes when a desired degree of convergence in energy is reached, which means that an *ad hoc* value for the relative energy change between two steps has to be decided previously in order to decide that the solution has been achieved.

III. RESULTS AND DISCUSSION

Figure 1 can not be reproduced with the numerical calculation performed in this work due to the fact that the energy that results from this method once the number of particles in the condensate exceeds the critical value N_{cr} is nonsense. That is because, unlike the variational approach, the code operates only under equilibrium conditions and it is not the case when the condensate has collapsed. When that happens, all the condensate density is concentrated in a central bin of the spatial mesh discretization, resulting in what looks like a Dirac delta function. That means that all the particles are in a single point, which can by no means be an equilibrium situation.

However, the results extracted from the numerical method explained in section II C can be compared to the ones derived from the variational method of section II B by means of the graphic plotted in Figure 2.

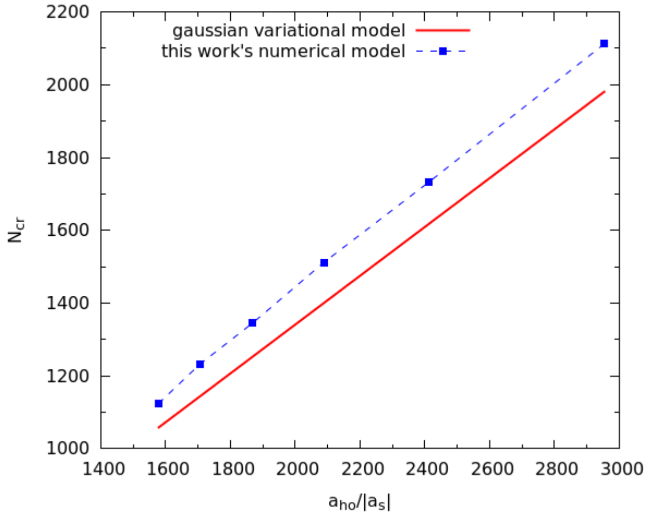

Figure 2: Comparison between the theoretical variational model (in red) and the numerical calculation performed in this work (blue squares connected with dashed lines). Critical number of bosons in the condensate N_{cr} as a function of its characteristic length a_{ho} divided by the absolute value of s-scattering lenght a_s.

Figure 2 shows the critical value of the condensate N_{cr} before it collapses as a function of an adimensional parameter $a_{ho}/|a_s|$. It is done in this way in order to compare the variational result to the numerical calculation performed in this work. As expected from (10) the variational model gives a straight line with a slope of approximately 0.6706. The numerical results have also a linear behavior but have a slightly different slope, which results to be 0.7127.

One can also see that the variational formula underestimates in about 5% the critical number of bosons that can fit in the condensate before it collapses given a_{ho}/a_s. This is because the Gaussian function it uses is a good representation of the cloud roughly speaking, but the real function that describes correctly the cloud is slightly broader. For this reason, the numerical calculation, which allows that the *trial function* has more degrees of freedom, is closer to the correct description of the system and gives a larger number of bosons under the same conditions.

In Figures 3 and 4 the variational and the numerical solutions are plotted for lithium-7 atoms in three dimensional harmonic traps of two different frequencies. One can see that while both the variational Gaussian function and the one that is used in this calculation are very similar, the first is slightly narrower than the last.

This agrees with the fact that the variational method underestimates the number of bosons that fit in the condensate, as the square modulus of the wave function can be related to the cloud density.

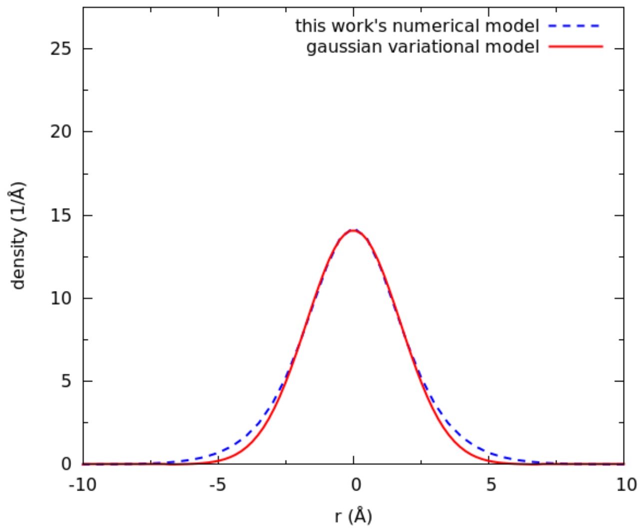

Figure 3: Comparison between the Gaussian trial function that the variational method uses (in red) and the numerical function (in dashed blue) for a mean oscillator trap frequency of ω_{ho} =75 Hz. For this frequency the variational approach gives a N_{cr} of 1617 bosons while the numerical calculation gives 1732 as the maximum of particles the condensate can hold.

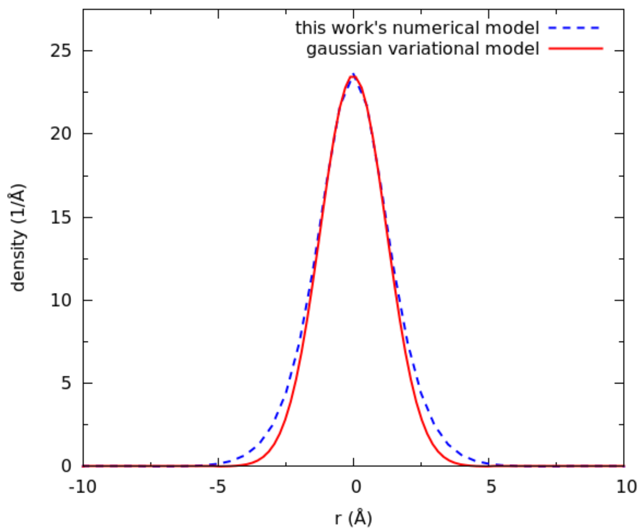

Figure 4: Another comparison between the Gaussian trial function that the variational method uses (in red) and the numerical function (in dashed blue) for ω_{ho} =175 Hz. For this frequency the variational approach gives an N_{cr} of 1058 bosons while the numerical calculation gives 1125.

IV. CONCLUSIONS

This work has studied two different ways of obtaining the critical number of atoms in a trapped dilute Bose-Einstein Condensate with attractive weak interactions between the atoms at zero temperature. The expression based on a variational method [1] has been proved to be of a good quality in a coarse way. However, it happens to underestimate this value due to the fact that the Gaussian Function that this approach uses as a trial wave function is slightly narrower than the real density. Instead, the numerical method studied in this work is a better approximation to the experimental density because it allows the trial function to have more degrees of freedom. Thus, the critical number of particles in a condensate obtained from this last method is supposed to be closer to the experimental value.

Acknowledgments

I would like to express my deep gratitude to Professor Ricardo Mayol, my supervisor, for his patient guidance, enthusiastic encouragement and useful critiques of this work. Adrià Moreno deserves special acknowledgment for his assistance and comments about this work. Finally, I wish to thank my parents for their support and encouragement throughout my study.

[1] Franco Dalfovo, Stephano Giorgini, Lev P. Pitaevskii, Sandro Stingari. *Theory of Bose-Einstein condensation in trapped gases.* Rev. Mod. Phys., Vol.71, No. 3, April 1999

[2] A. Griffin, D. W. Snoke, and S. Stringari, *Bose-Einstein Condensation* (Cambridge University Press, Cambridge (1995)

[3] M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman and E. A. Cornell *Observation of Bose-Einstein Condensation in a Dilute Atomic Vapour* Science **269**, 198 (1995)

[4] K. B. Davis, M. O. Mewes, M. R. Andrews, N. J. van Druten, D. S. Durfee, D. M Kurn and W. Ketterlee, *Bose-Einstein Condensation in a Gas of Sodium Atoms* Phys. Rev. Lett **75**, 3969 (1995)

[5] C.A. Sackett, C.C. Bradley, M. Welling, R.G. Hulet, *Bose-Einstein condensation of lithium* Appl. Phys. B **65**, 433-440 (1997)

[6] C. J. Pethick, H. Smith, *Bose-Einstein Condensation in Dilute Gases*, chap 4, Cambridge University Press (2001)

[7] B.H. Bransden, C.B. Joachin, *Physics of Atoms and Molecules* Prentice Hall, 2nd ed. (2002)

[8] Cheng Chin, Rudolf Grimm, Paul Julienne, Eite Tiesinga, *Fesbach ressonances in ultracold gases* Rev. Mod. Phys. **82,** 1225 (29 April 2010)

[9] Gordon Baym, C.J. Pethrick. *Ground-State Properties of Magnetically Trapped Bose-Condensated Rubidium Gas* Phys. Rev. Lett. **76** (1996)

[10] K.T.R. Davies, H. Flocard, S. Krieger, M.S. Weiss. *Application of the imaginary time step method to the solution of the static Hartree-Fock problem* LBL-10269, 1980