SINGULARITY FORMATION AND COLLAPSE IN THE ATTRACTION
GROSS-PITAEVSKII EQUATION

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A generic mechanism of collapse in the Gross-Pitaevskii equation with attractive interparticle interactions is gained by reformulating this equation as Newton’s equation of motion for a system of particles with a constraint. ‘Quantum pressure’ effects give rise to formation of a potential barrier around the emerging singularity, which prevents a fraction of the particles from falling into the singularity. For reasonable initial widths of the condensate, the fraction of collapsing particles, which are thereby removed from the condensate, is found to be a ‘universal’ number \( \simeq 0.7 \).

The Bose-Einstein condensate formed in a magneto-optically trapped vapor of cold alkali atoms, can be quite accurately described by the Gross-Pitaevskii (GP) equation [1]

\[
\frac{i}{\hbar} \frac{\partial}{\partial t} \psi + \frac{\hbar^2}{2m} \Delta \psi - g |\psi|^2 V(x) \psi = 0, \quad (1)
\]

where \( \psi(x, t) \) is the wave function of the condensate, the external potential \( V(x) \) models the wall-less confinement (the trap), \( m \) is the mass of an individual atom, \( g = 4 \pi \hbar^2 a_s / m \) is the effective interaction strength (the ‘coupling constant’) with \( a_s \) the scattering length, and \( \Delta = \sum_i \frac{\partial^2}{\partial x_i^2} \) is the Laplace operator. A convenient as well as practical choice for the confining trap is the paraboloidal potential \( V = \frac{m}{2} \sum_i \omega_i^2 x_i^2 \).

It has been known [2] that for some while already that the Bose-Einstein condensate of atoms with a negative scattering length becomes unstable when the number of atoms exceeds some critical value \( N_c \). These instabilities have recently been analyzed experimentally. To this end the most interesting prospects are provided by the application of Feshbach resonance by which one can actually tune the effective scattering length with an external magnetic field, and thereby e.g. sweep the coupling constant from positive to negative. This technique was very recently used [3] on a condensed gas of \(^{85}\)Rb atoms such that a collapse and the consequent ‘explosion’ of a condensate of \(^{85}\)Rb atoms was created.

Triggered by these recent experiments, a possible mechanism through elastic collisions for the ejection from the condensate of atoms with negative scattering length was discussed in [4]. In this Letter we show however that the mean-field theory (i.e. the GP equation) of the condensate already allows for a description of ‘partial collapse’, and leads to an accurate estimate for the number of particles that remain in the condensate after the explosion. The fraction of the condensate thrown away in the collapse (i.e. the collapsing part of the condensate), is always about 70% provided that the width of the condensate before the change of sign of the scattering length is close to that of the ground state. This was true e.g. for the experiment reported in [5]. We find that the collapsing fraction is relatively insensitive to the total number of particles in the condensate, and that this fraction tends to 100% only in the limit of very large width of the condensate.

Collapse phenomena are very well known in nonlinear optics and plasma physics, and they have there a long history extending over the last thirty years (see e.g. review [6] and references therein). Following this tradition, the collapse in the GP system with a negative scattering length was discussed in a similar fashion in [7–9].

Within this tradition, the analysis of singularity formation is mainly focussed on the self-similar behaviour of the solutions in the vicinity of the singularity. We have recently shown [10], however, that a true self-similar solution of the GP system is only possible in two space dimensions. This means that a self-similar description of collapse can only be used with certain reservations. In this Letter we propose a completely different description for the singularity formation, which does not rely on self-similarity of the solution. In a sense the starting point of our analysis is the concept of ‘partial collapse’, now of the Bose-Einstein condensate. A suggestion about a singularity restricted to a localized domain inside the condensate, was already made in [9]. Here we elaborate further on this suggestion, and formulate it within a completely different framework from that used in [10].

Our approach is based on the realization that the GP equation Eq. (1) can be interpreted as Newton’s equations of motion for (fictitious) particles with a certain constraint. The dynamics of GP collapse can then easily be followed by following the trajectories of these particles, under the influence of an effective potential due to ‘pressure’ effect that arise from the spatially varying condensate density. By introducing an auxiliary field \( \eta(x, t) \), and its inverse \( r(\eta, t) \), we can show (see below) that these trajectories satisfy a system of ordinary differential equations,
\[
\frac{\partial \rho_i}{\partial t} = \frac{1}{m} \frac{\partial \phi}{\partial x_i} (r(\eta, t), t); \quad r_i(\eta, 0) = \eta_i,
\]
with \( i = 1, 2, 3 \) for \( d=3 \) dimensions. Here \( \phi \) is a phase defined by the representation \( \Psi = \sqrt{\rho e^{i\phi}/\hbar} \) of the condensate field. The fields \( r_i(\eta, t) \) can now be interpreted as trajectories of some particles with initial points \( \eta_i \). We describe in the following how the GP equation Eq. (1) can be transformed into the equations of motion for this system of particles.

It is plain that, by using \( \Psi = \sqrt{\rho e^{i\phi}/\hbar} \), Eq. (1) is equivalent to a coupled set of equations for \( \rho \) and \( \phi \),

\[
\rho_t + \frac{1}{m} \text{div}(\rho \nabla \phi) = 0
\]

for all \( \eta \in \Omega \). In other words, all particle trajectories that begin at any \( \eta \in \Omega \) are converged at one point \( r_\ast \), i.e., \( \rho(r_\ast, t_\ast) = \infty \). Then, from Eq. (11), we can conclude that for any \( r_\ast \) there is a set \( \Omega_\ast \) such that

\[
\lim_{t \rightarrow t_\ast} r_i(\eta, t) = r_{si}
\]

for all \( \eta \in \Omega_\ast \). In other words, all particle trajectories that begin at any \( \eta \in \Omega_\ast \) are converged at one point \( r_\ast \).
Suppose that the set of singular points, \( \{ r_s \} \), consists of one isolated point while \( \Omega_s \) is a domain. We can then define the number of particles involved in the collapse as

\[
N_e = \int_{\Omega_s} \rho_0(\eta)d^3\eta.
\]

This number can thus be interpreted as the number of particles that are ejected from the condensate when it is collapsed. Notice that the domain \( \Omega_s \) can also coincide with the whole space. In this case \( N_e = N \), the total number of atoms in the condensate. This is true in particular for the self-similar solutions, when the whole condensate collapses to a \( \delta \)-function centered in the trap, and completely disappears apart from the very particular borderline case of an oscillating solution [15]. The self-similar solutions can only exist [13] in two space dimensions. It is important to emphasize that, in general, \( N_e < N \). It can be shown, e.g., that if \( \rho_0 \) tends to a Gaussian distribution as \( |\eta| \to \infty \), then \( N_e < N \). This means that \( N_e \) is an essential characteristics of the collapse of attractive condensates.

We can explain the partial collapse qualitatively as follows. If, initially, the width of the condensate is greater than the characteristic oscillator length \( a_{HO} \), both the quantum pressure and the conventional pressure induce the condensate to decrease its width. However, when the width becomes equal or less than \( a_{HO} \), the two pressure terms in the energy have opposite effects: quantum pressure favours an expanding condensate (as a result of an ‘uncertainty principle’), while the negative conventional pressure term favours a collapsing condensate. Provided that the number of particles is greater than a critical value, the negative pressure dominates over the quantum pressure in a small domain centered at a point \( r_s \). Outside this domain it is the quantum pressure that dominates, and prevents the outside particles from entering this domain.

In order to estimate the value of \( N_e \), we use here a Gaussian trial wave function [17–20]. It gives an approximate solution for the density, which can be expressed in the form

\[
\rho(x, t) = \frac{N}{\pi^{3/2}} \prod_i \tau_i(t)^{-1} e^{-\sum_i \frac{r_i^2}{\tau_i(t)}},
\]

in which the functions \( \tau_i \) satisfy [21–23]

\[
\frac{\dot{\tau}_i}{\tau_i} + \frac{\hbar^2}{m^2 \tau_i^3} - \frac{gN}{(2\pi)^{3/2}m} \prod_i \frac{1}{\tau_i} = 0
\]

with \( \tau_i(0) = a_i \) and \( \dot{\tau}(0) = 0 \). Here \( a_i \) is the initial width of the condensate.

Substituting the solution Eq. (15) in Eq. (8), we find that

\[
\frac{\partial^2 \dot{\tau}_i}{\partial t^2} = -\frac{\partial V_{\text{eff}}}{\partial \tau_i},
\]

\[
V_{\text{eff}}(r, t) = \frac{1}{2} \sum_i \left( \frac{\hbar^2}{m^2 \tau_i^2} \right) \dot{\tau}_i^2 + \frac{g}{m} \rho(r, t).
\]

Here \( V_{\text{eff}} \) is an effective time-dependent potential that determines the behaviour of particle trajectories in the vicinity of the center of the trap.

For simplicity, we consider here in more detail the symmetric trap: \( \omega_i = \omega \) and \( a_i = a \). Hereafter we measure the time in units of \( 1/\omega \), and the distance in units of \( a_{HO} = \sqrt{\hbar/m\omega} \), the oscillator length. Now Eqs. (17), (18) take the form

\[
\frac{d^2\tau_i}{dt^2} = -\frac{\partial V_{\text{eff}}}{\partial \tau_i},
\]

\[
V_{\text{eff}} = \frac{1}{2} \left( 1 - \frac{1}{\tau_i^2} \right) r_i^2 - \frac{4}{\sqrt{\pi}} \frac{g_0}{\tau_i^3} \left( e^{-\frac{r_i^2}{\tau_i^2}} - 1 \right),
\]

and

\[
\frac{d^2\tau}{dt^2} + \frac{1}{\tau^3} + \frac{2 g_0}{\sqrt{\pi} \tau^4} = 0,
\]

in which \( g_0 = \frac{|\omega| N}{a_{HO}} \) and the initial conditions are given by \( r(0) = \eta, \dot{r}(0) = 0, \tau(0) = a, \dot{\tau}(0) = 0 \). Notice that if \( g_0 > g_{\text{cr}} \), where \( g_{\text{cr}} \approx 0.671 \) [1], the solution of Eq. (19) has a zero at a finite time \( t = t_* \).

![FIG. 1. The effective potential \( V_{\text{eff}} \) at different times \( t < t_* \). The initially almost paraboloidal potential develops a growing barrier at the final stages of the collapse.](image)

Let us assume that the system has \( a > 1 \) and begins to collapse. Initially, \( V_{\text{eff}} \) can be well approximated by a paraboloidal trap. The particles are drifted towards the center and the condensate width decreases. When this width is reduced to the oscillator length, a potential barrier is however formed at a distance \( r = r_{\text{max}} \) from the center,

\[
r_{\text{max}} = \tau \sqrt{\ln \frac{8 g_0}{\sqrt{\pi} (\tau - \tau^5)}},
\]

preventing the outside particles from falling into the emerging singularity. Figure 1 illustrates the formation
of this potential barrier in the limit when the width of the condensate \( \tau \) goes to zero.

We solved the system Eqs. (18), (19) numerically. The collapse time was obtained from the condition \( \tau(t_*) < 0.1 \). Equation (18) was solved in the time interval \([0, t_*)\), while the point \( \eta \) was supposed to belong to the domain \( \Omega_s \) provided that \( r(t_*) < r_{\text{max}}(t_*) \).

The conditions of the experiment reported in \([1,2]\) were modelled such that the initial width of the condensate was derived as a stationary solution of Eq. (19) with \( g_0 \) replaced by \(-41.67g_0\). Notice that in the experiment \([1,2]\) the initial positive scattering length was \(2500a_0\), which we proposed here, is not accurate if the 'coupling constant' \(g_0\) is in the vicinity of \(g_{\text{cr}}\). The simplified model based on Gaussian trial wave function, which we proposed here, is not accurate if the 'coupling constant' \(g_0\) is in the vicinity of \(g_{\text{cr}}\). More thorough analysis of Eq. (1) will be reported in a forthcoming publication.

\(^{1}\)The final stage of the collapse takes place very fast, so a good numerical estimate for \(t_\ast\) was already obtained from this seemingly rather crude approximation, which however allowed us to avoid the difficulties related to the mathematical singularity at \(t = t_\ast\).