Singularity formation in the Gross-Pitaevskii Equation and Collapse in BEC

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We study a mechanism of collapse of the condensate wave function in the Gross-Pitaevskii theory with attractive interparticle interaction. We reformulate the Gross-Pitaevskii equation as Newton’s equations for the particle flux and introduce a collapsing fraction of particles. We assume that the collapsing fraction is expelled from the condensate due to dissipation. Using this hypothesis we analyze the dependence of the condensate collapse on the initial conditions. We found that for a properly chosen negative scattering length the remnant fraction becomes larger when the initial aspect ratio is increased.

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I. INTRODUCTION

Collapse phenomena in Bose-Einstein condensates received a great deal of interest in the last few years Refs.[1, 2, 3, 4, 5, 6, 7, 8]. The experimental technique based on a Feshbach resonance allows to tune, through application of an external magnetic field, the strength of the interatomic interaction and even switch between repulsive and attractive interactions[6]. The realization of a collapse controlled by the magnetic field on a gas of $^{85}\text{Rb}$ reveals a rich dynamical properties of the collapsing condensates Ref.[11].

When the number of atoms becomes sufficiently large, the interatomic energy overcomes the quantum pressure and the condensate implodes. In the course of the implosion stage the density increases in the small vicinity of the trap center. When the density approaches certain critical values a fraction of the atoms gets expelled. In a time period of an order of few milliseconds the condensate stabilizes. There are two observable components in the final stage of the condensate dynamics: remnant and burst atoms. The remnant atoms are the atoms which remain in the condensate. The burst atoms have the energy which is much larger then the energy of the condensed atoms. There is also a fraction of atoms, which is not observable. This fraction is referred to as missing atoms. To account for dissipative losses in the collapse phenomena, the most part of theoretical studies reflected in existing literature try to modify the mean field theory through addition of damping terms modelling the mechanism of dissipative losses in the system. In particular, the results of experiment of Ref.[10] have been analyzed by numerical solution of the Gross-Pitaevskii (GP) equation with three body recombination term Refs.[11, 12, 13]. A mechanism of losses through elastic collisions was discussed in Ref.[3].

The References [11, 12] follow the ideas of experimental work [10] and obtain the burst atoms fraction fitting the Gaussian distribution to the condensate wave function. The essence of the approach of Refs. [11, 12] is the idea that the final state of the condensate is comprised of the remnant fraction surrounded by a very dilute fraction of burst atoms. Hence, the only fraction which is expelled from the condensate is that of the missing atoms, while the burst atoms fraction is formed in the course of the condensate dynamics.

Effective workings of a nonlinear mechanism of dissipation in description of collapse in BEC are inherently connected to the structure of singularity [15] which is formed in the course of the nonlinear dynamics as described by the Gross-Pitaevskii equation [1]. This equation reads

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

Here $\Psi(x,t)$ 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, $g = 4\pi\hbar^2m^{-1}a_s$ is the effective interaction strength (the ‘coupling constant’), $a_s$ is 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 $V = \frac{\hbar^2}{2m} \sum_i \omega_i^2 x_i^2$. Notice that so far very little is known about the singularity structure of the 3D GP equation Eq.(1) outside treatments of spherically symmetric case (see the monograph [16] and references therein). In this work we will try to gain an insight into the problem through reformulation of the Gross-Pitaevskii equation Eq.(1) in a different form. Our approach resembles, at least formally, the de Broglie-Bohm formulation of quantum mechanics [17, 18].

We introduce quantum trajectories ($q$-trajectories) of the GP equation Eq.(1). These trajectories satisfy a system of ordinary differential equations, viz.

\[ \frac{\partial r_i}{\partial t} = \frac{1}{m} \frac{\partial \phi}{\partial x_i} \mathbf{r}(\eta, t); \quad \mathbf{r}_i(\eta, 0) = \eta_i, \] (2)

with $i = 1, 2, 3$ in the 3D case. Here $\phi$ is the 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 the fictitious particles with the initial points located at $\eta_i$. These trajectories satisfy the Newton equations of motion for a set of particles,

$$m \frac{\partial^2 r_i}{\partial t^2} = -\frac{\partial V}{\partial x_i} - \frac{\partial U}{\partial x_i},$$

where the 'pressure potential' $U(x, t)$ is

$$U(x, t) = -\frac{\hbar^2}{2m} \rho^{-1/2} \Delta \rho^{1/2} + g \rho.$$

In addition, the Liouville formula for Eq. (2) can be written in the form

$$\det \left( \frac{\partial r_i}{\partial \eta_k} \right) \rho(r, t) = \rho_0(\eta),$$

where $\rho_0$ is the initial density of the condensate. The system of equations Eqs. (3), (5) is equivalent to the original GP equation Eq. (1).

As was indicated above the $q$-trajectories are used in the de Broglie-Bohm causal interpretation of quantum mechanics Refs. [17, 18]. In our previous work Ref. [19] we employed these trajectories to define singularities of the GP equation Eq. (1). Indeed, Eq. (5) immediately suggests that a set of singular points $r_s$ of the GP equation Eq. (1) at which $\rho(r_s, t_s) = \infty$ for some fixed $t_s$ in terms of $q$-trajectories, describes either the caustic or focal points of the trajectories. Notice that in the case of linear Schrödinger equation the probability density $\rho$ is always finite and caustics do not exist.

The Newton equations Eqs. (3) define the flux of particles. The appearance of the burst atoms in the mean field theory can be qualitatively understood through analysis of the energy distribution near the singularity in the flux of particles as shown in Figure 1. In this picture the peak with positive energy density arises due to the acceleration of the particles by the singularity. This acceleration is proportional to $g \nabla \rho$ and results in increase of the kinetic energy of the particles surrounding the singularity. In Figure 1 the curves with greater peaks correspond to the moments of time closer to $t_s$. The burst atoms can be formed only if the dissipation losses occur faster than the collapse domain is refilled by the flux. In this case one observes intermittent implosions as reported in Ref. [1].

The burst atoms cannot appear in the framework of the mean field theory if the damping parameter is chosen to be large enough (cf. Ref. [13]). In this case the density cannot increase to sufficiently large values and the peak of the positive energy density is not formed.

The dynamics of the $q$-trajectories which begin at the points located far from the origin in the $\eta$-space cannot be significantly affected by possible dissipative term. This is because the compression of the breathing mode of the harmonic oscillator, which is $1/4$ of the period of the oscillator, is of the same order of magnitude as the time of the collapse including the time of dissipation. This means that the remote trajectories cannot reach the collapse domain.

In the presence of the burst atoms the condensate dynamics outside the dissipation domain is a quite complicated interference of the ‘outgoing’ burst atoms and ‘incoming’ atoms. Should we neglect this interference, the fraction of the remaining atoms could be found through the analysis of the particles flux falling into the singularity and described by the Newton equations Eqs. (3). Notice that these equations are still valid in the presence of dissipative term. However in this case the relation Eq. (1) does not hold.

The analysis of flux of particles falling into the singularity shows that the fraction of atoms remaining in the condensate is consistently constant for the wide range of parameters. This effect is supported by an experimental evidence [4]. In this work we deal with the general case of asymmetric trap. In our previous work Ref. [14] we reported for the symmetric trap an effect similar to the described above. Our computation was based on a Gaussian trial wave function which was used to estimate a part of atoms focusing on the caustic. Here we discuss different types of collapse which can exist in asymmetric trap.

The paper is organized as follows. In the next section we discuss different types of collapse which can oc-
cur in the asymmetric trap. In the section 3 we obtain the collapsing fraction and show that this fraction in the broad range of parameters consistently remains almost constant.

II. BREATHING MODE OF THE CONDENSATE

In this section we consider types of collapse which can be observed in an asymmetric trap. We use as the initial condition the Gaussian profile. For this profile

\[ \rho_0 = \frac{N}{\pi^{3/2}} \prod_{i=1}^{3} \frac{1}{w_i} e^{-x_i^2/w_i^2} \]

the harmonic oscillator equation has explicit solution, viz.

\[ r_i(\eta, t) = \sigma_i(t) \eta_i, \quad (i = x, y, z) \]

where

\[ \sigma_i(t) = \sqrt{\cos^2(\omega_i t) + \frac{a_i^4}{w_i^2} \sin^2(\omega_i t)}, \quad a_i = \frac{\hbar}{m \omega_i} \]

It seems natural, at least for Gaussian initial conditions, to expect that the breathing mode described by Eq. (3) gives the main contribution into the action

\[ S(r) = \int dt \int d\eta \rho_0(\eta) \mathcal{L}, \]

where

\[ \mathcal{L} = \sum_{i=1}^{3} \frac{m}{2} \dot{r}_i^2 - \frac{\hbar^2}{2m} (\nabla \sqrt{\rho})^2 - V - \frac{g}{2} \rho. \]

This provides us with the motivation to employ the variational principle and to seek for the solution of the GP equation Eq. (4) in the form \( r_i(\eta, t) = \tau_i(t) \eta_i \). Substituting this into the action we obtain

\[ \ddot{\tau}_i + \omega_i^2 \tau_i - \frac{\hbar^2}{m^2} \tau_i - \frac{gN}{(2\pi)^{3/2}m} \prod_k \tau_k \tau_i = 0 \quad (i = x, y, z) \quad (7) \]

The density as obtained through the relation Eq. (5) reads

\[ \rho(x, t) = \frac{N}{\pi^{3/2}} \prod_{i=1}^{3} \frac{1}{\tau_i} e^{-x_i^2/\tau_i^2} \quad (8) \]

Here we have included \( w_i \) in \( \tau_i \) and used \( \rho_0 \) with \( w_i = 1 \).

The result Eq. (8) is well-known Gaussian trial wave function Ref. [20]. This function describes the breathing (monopole) mode of the condensate.

In what follows we measure the time in units of \( 1/\omega \), where \( \omega = (\omega_x \omega_y \omega_z)^{1/3} \), and the distance in units of the oscillator length \( a_{HO} = \sqrt{\hbar/m \omega} \). For the axial symmetric equation we have \( \omega_x = \omega_y = \omega_z \) and \( \tau_x = \tau_y = \tau_z \). Then the system Eqs. (7) is reduced to the following equations

\[ \ddot{\tau}_x + \beta^2 \tau_x - \frac{1}{\tau_x} - \sqrt{\frac{2}{\pi}} \frac{\kappa}{\tau_x^2} \tau_x = 0 \quad (9) \]

\[ \ddot{\tau}_r + \frac{1}{\beta} \tau_r - \frac{1}{\tau_r^3} - \sqrt{\frac{2}{\pi}} \frac{\kappa}{\tau_r^2} \tau_r = 0 \quad (10) \]

Here \( \beta = \frac{\omega}{\omega_0} \) and \( \kappa = \frac{Na_0^3}{m^2} \).

For negative \( \kappa \), such that \( |\kappa| \) is greater than certain critical value, the system of Eqs. (9), (10) has singular solutions with \( \tau_r \rightarrow 0 \) as \( t \rightarrow t_\ast \). We found three different regimes of collapse.

Spherically symmetric collapse is characterized by \( \tau_z \sim \tau_r \sim t \rightarrow t_\ast \). The functions \( \tau_r, \tau_z \) near the singularity are described by the power law

\[ \tau_z \sim \tau_r \sim (t_\ast - t)^{1/2}, \quad \tau_r \sim (t_\ast - t)^{1/5} \]

where \( t_\ast \) is some constant. In this regime the compression of the condensate is uniform in all directions.

Radial collapse is effectively two dimensional collapse for which the condensate contracts only in the radial direction. The behavior of \( \tau_z, \tau_r \) near \( t_\ast \) is defined by

\[ \tau_z \sim \lambda, \quad \tau_r \sim (t_\ast - t)^{1/2}. \quad (11) \]

Here \( \lambda \) is a constant and \( t_\ast = \sqrt{2} \left( \frac{\sqrt{2} \sqrt{|\kappa|} - 1}{\sqrt{2} \sqrt{|\kappa|} - 1} \right)^{1/4} \).

Axial collapse is characterized by \( \tau_z \sim \tau_r^3 \) as \( t \sim t_\ast \).

In this case the compression of the condensate is faster in the axial direction. The function \( \tau_z \) approaches zero through an oscillating regime. This regime cannot be described by a power law.

The actual type of singularity depends on the initial conditions for Eqs. (7), (10). To begin the analysis we specify the parameters and initial data as \( \beta = 0.5325, \tau_z(0) = 0, \tau_r(0) = 0, \tau_x(0) = \tau_{0a} \) and \( \tau_y(0) = \tau_{0a} \).

The constants \( \tau_{0a}, \tau_{0a} \) are a stationary solution of the system of Eqs. (7), (10) with \( \kappa = \kappa_{in} > 0 \). This choice of parameters models experiments on Feshbach resonances when the scattering length is instantly changed from positive to negative values in the initial stage of the dynamics.

For accurate implementation of numerical simulation we use the following change of variables

\[ \tau_z = e^{\nu_z(\theta)}, \quad \tau_r = e^{\nu_r(\theta)}, \quad \theta = \ln \frac{t_c}{t_c - t}, \]

where \( t_c \) is a constant. The functions \( \nu_r, \nu_z \) are regular in the interval \( [0, +\infty) \) if \( t_c \leq t_\ast \) and acquire a singularity at some \( \theta_s < +\infty \) if \( t_c > t_\ast \).

We also obtain \( \lambda \) as a function of \( \kappa, \kappa_{in} \) as shown in Figure 4. In this Figure the open domain \( \Omega_{\lambda} \) in \( \kappa - \kappa_{in} \) plane consists of two disconnected components.
The overall domain $\Omega_{\lambda}$ corresponds to the radial collapse. The component $\Omega_{\lambda}^{(1)}$ corresponds to the simple radial collapse. In this subdomain the attraction between atoms is strong, i.e. $|\kappa|$ is large. This results in fast and monotonous decreasing of the Gaussian widths $\tau_i$, $i = x, y, z$. Notice that while $\tau_{x,y}$ vanish, $\tau_z$ remains finite as in Eq. (11). In the second component of $\Omega_{\lambda}$, i.e. in $\Omega_{\lambda}^{(2)}$ the density $\rho(0,t)$ has at least one local maximum in the interval $(0, t_*)$. In this regime the collapse occurs after a regular compression-expansion cycle. The rates of contraction in the radial and axial directions are alternating with each other in magnitudes. At some instances an intensive contraction in one direction is compensated by expansion in the other. Notice that the final stage of this process is always the contraction in the radial direction. This is why we refer to this type of collapse as to the radial collapse. We turn next to the description of the open domain complimentary to the domain $\Omega_{\lambda}$ in the $\kappa - \kappa_{in}$ plane. This is the groove shown in Figure 2. This domain corresponds to the axial collapse. In the case of axial collapse the ultimate stage of the dynamics is always the faster contraction in the axial direction. A typical behavior in axial collapse is shown in Figure 3.

The boundary separating the open domain $\Omega_{\lambda}$ and the groove, i.e. $\partial\Omega_{\lambda}$ corresponds to the spherically symmetric collapse. It is interesting to notice that even though the trap is asymmetric, the workings of nonlinear dynamics still allow the spherical collapse to occur.

Intuitively, the existence of a regular cycle in dynamics of the breathing mode for $(\kappa, \kappa_{in}) \in \Omega^{(2)}$ suggests that fewer number of atoms must be removed to stabilize the condensate. We further discuss this idea in the next section where we analyze the flux of particles.

\[ \Omega^{(1,2)}_{\lambda} = \Omega^{(1)}_{\lambda} \cup \Omega^{(2)}_{\lambda} \] located on the different sides of the groove. The overall domain $\Omega_{\lambda}$ corresponds to the radial collapse. The component $\Omega^{(1)}_{\lambda}$ corresponds to the simple radial collapse. In this subdomain the attraction between atoms is strong, i.e. $|\kappa|$ is large. This results in fast and monotonous decreasing of the Gaussian widths $\tau_i$, $i = x, y, z$. Notice that while $\tau_{x,y}$ vanish, $\tau_z$ remains finite as in Eq. (11). In the second component of $\Omega_{\lambda}$, i.e. in $\Omega^{(2)}_{\lambda}$ the density $\rho(0,t)$ has at least one local maximum in the interval $(0, t_*)$. In this regime the collapse occurs after a regular compression-expansion cycle. The rates of contraction in the radial and axial directions are alternating with each other in magnitudes. At some instances an intensive contraction in one direction is compensated by expansion in the other. Notice that the final stage of this process is always the contraction in the radial direction. This is why we refer to this type of collapse as to the radial collapse. We turn next to the description of the open domain complimentary to the domain $\Omega_{\lambda}$ in the $\kappa - \kappa_{in}$ plane. This is the groove shown in Figure 2. This domain corresponds to the axial collapse. In the case of axial collapse the ultimate stage of the dynamics is always the faster contraction in the axial direction. A typical behavior in axial collapse is shown in Figure 3.

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III. THE FLUX OF PARTICLES

The $q$-trajectories $r_i(\eta, t) = \tau_i \eta_i$ derived in the previous section focus at the symmetry axis when the time approaches $t_*$ for any $\eta$. However, for the large $|\eta|$ this is not true, since in this region the behavior of the function $r(\eta, t)$ is determined by the solution of the harmonic oscillator equation Eq. (8).

The scope of analysis of equations for quantum trajectories Eqs. (9) proposed in this section attempts go beyond the limitations posed by the Gaussian ansatz. In what follows we construct an effective approximation for the flux of particles. Our approximation effectively uses the notion of quantum trajectories. We gain a motivation for this approach from the analysis of the quasi-classical approximation for the Schrödinger equation. To construct the quasi-classical approximation of the Schrödinger equation we have to solve the Newton equations for the trajectories of particles, i.e. to solve $\dot{r}_i = -\alpha \frac{\partial V}{\partial r_i}$. The amplitude and the phase of the wave function are determined through Eqs. (9). We can search further corrections substituting the quasi-classical amplitude into the Newton equations Eqs. (9) with $g = 0$. Iterating this procedure and assuming that iterations converge we finally get the solution of the Schrödinger equation in the time interval $[0, T]$ such that the function $r(\eta, t)$ with $t \in [0, T]$ is invertible at each step. For instance, in the case of harmonic oscillator and Gaussian initial conditions this procedure converges in the interval defined by the inequality $\prod_{i} \cos(\omega_i t) > 0$. In fact we construct here an iteration procedure $F$ of the form $r^{(n)} = F(r^{(n-1)})$, where $n$ is the number of iteration. These iterations start from the trajectories of the classical harmonic oscillator $r_i^{(0)} = r_i^{(0)}(\eta, t) = \cos(\omega t)\eta_i$. Notice that the mechanism of the iteration procedure $F$
is disconnected from the quasi-classical approximation. This procedure is equally well applicable in both linear and nonlinear \((g \neq 0)\) cases. Indeed, solving Eqs. (3) in the nonlinear case, we can then find from Eq. (8) a next iteration for the function \(\rho\) which we again employ in Eqs. (3), and so forth.

Below we introduce an effective approximation for the quantum trajectories as the first step of the iteration procedure \(F\) described above. We assume that the starting solution Eq. (6) delivered by the variational principle is reasonably close to the exact solution. Using Eqs. (3) with the density given by equation Eq. (8) and substituting Eq. (5) into Eqs. (3), and so forth.

We now define the collapsing fraction of atoms by an integral

\[
\frac{\partial^2 r_i}{\partial t^2} = -\frac{\partial V_{eff}}{\partial r_i}, \quad r_i(0) = \eta_i, \quad \dot{r}_i(0) = 0, \tag{12}
\]

where

\[
V_{eff}(r, t) = \frac{1}{2} \sum_i \left( \frac{\omega_i^2}{\omega^2} - \frac{1}{\tau_i^2} \right) r_i^2 + 4\pi\kappa\rho(r, t)/N.
\]

Notice that for the case of an axially symmetric trap it is sufficient to consider the behavior of the \(g\)-trajectories in \(x-z\) plane. This can be achieved through reduction \(r_y = 0\).

At the moment of time \(t_c\) close to \(t_s\) we observe two main types of trajectories: the trajectories which go away from the center and the trajectories which tend to focus on the symmetry axis. The domain in the \(\eta\)-space corresponding to the focussing trajectories is denoted by \(\Omega_s\).

We now define the collapsing fraction of atoms by an integral

\[
N_c = \int_{\Omega_s} \rho_0 d\eta_i. \tag{13}
\]

Here \(\rho_0\) is the initial density. It is physically plausible to assume that the collapsing fraction is removed from the condensate due to the dissipation. Then the remaining fraction is given by the formula \(1 - N_c/N\).

We analyze numerically the flux of particles falling into the singularity. To do this we solve Eqs. (8), (10), (12). At the moment \(t = t_c\) the focussing trajectories with reasonable accuracy get inside the domain \(\Omega_s\). This domain is restricted by the ellipsoid of revolution of an ellipse with the semi \(x\) and \(z\)-axes equal \(\tau_z(t_c)\) and \(\tau_r(t_c)\) respectively. For \(t_c \rightarrow t_s\) the domain \(\Omega_s\) reduces to the interval \([-\lambda, \lambda]\) in the \(z\)-axis.

We now technically define the domain \(\Omega_s\) in the \(\eta\)-space such that if \(r(\eta, t_c) \in \Omega_s\) then \(\eta \in \Omega_s\). The results of simulations are presented in Figure 4. We find that the fraction \(N_c/N\) is consistently around 70% for large values of \(|\kappa|\) and depends neither on \(\kappa_{in}\) nor on \(N\). More exactly this is true for the subdomain \(\Omega_s^{(1)}\) corresponding to the simple radial collapse described above. The collapsing fraction decreases abruptly for \(|\kappa| < |\kappa_c|\), where \(\kappa_c\) is a certain threshold value specific to the given value of the parameter \(\kappa_{in}\). These thresholds for three different values of \(\kappa_{in}\) are shown in Figure 4. As was explained above, below the threshold \(|\kappa_c|\), in the domain \(\Omega_s^{(2)}\) and in the groove, we observe oscillatory dynamical patterns. In the course of these oscillations we observe losses in the collapsing fraction. For large \(\kappa_{in}\) and in this region the fraction \(N_c/N\) is found to be around 20%.

\[\text{FIG. 4: The fraction } N_c \text{ as a function of } |\kappa| \text{ for three different values of } \kappa_{in}.\]

IV. CONCLUSIONS

In this paper we suggest a simple model Eq. (12) of the BEC collapse based on the dynamical properties of the GP equation. Our model is independent of the damping parameter and a microscopic mechanism of the atom ejection. In the framework of this model it is impossible to correctly interpret the burst atoms fraction. However, the simplicity of the model allows us to study the problem in wide range of the parameters.

Using the notion of the flux of particles we define the collapsing fraction \(N_c\) as the part of atoms focusing at the symmetry axis. This focusing results in infinite increase of the density. Because of this we assume that total collapsing fraction is removed from the condensate. We estimate that \(N_c/N = 0.7\) for sufficiently large \(\kappa\) and the remaining fraction in this case is insensitive to the choice of parameters. Interestingly, our results show that changing the initial aspect ratio by \(\kappa_{in}\) it is possible to move from the domain \(\Omega_s^{(1)}\) to the domain \(\Omega_s^{(2)}\) for the same interaction strength \(\kappa\). This means that the fraction of remaining atoms can be increased for the larger initial aspect ratio controlled by \(\kappa_{in}\). In our opinion this effect deserves experimental investigation.
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