

Collapse of gaseous Bose-Einstein condensates and generation of non-condensate atoms

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Scientific School "Nonlinear Waves - 2020" March 2, 2020

Nizhny Novgorod, Russia

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OUTLINE

- Introduction: history and experimental data
- Main goals
- Collapse in Thomas-Fermi approximation
- Linear stability of strong collapse
- Weak collapse and its stability
- Conclusion and open questions

Introduction: history and experimental data

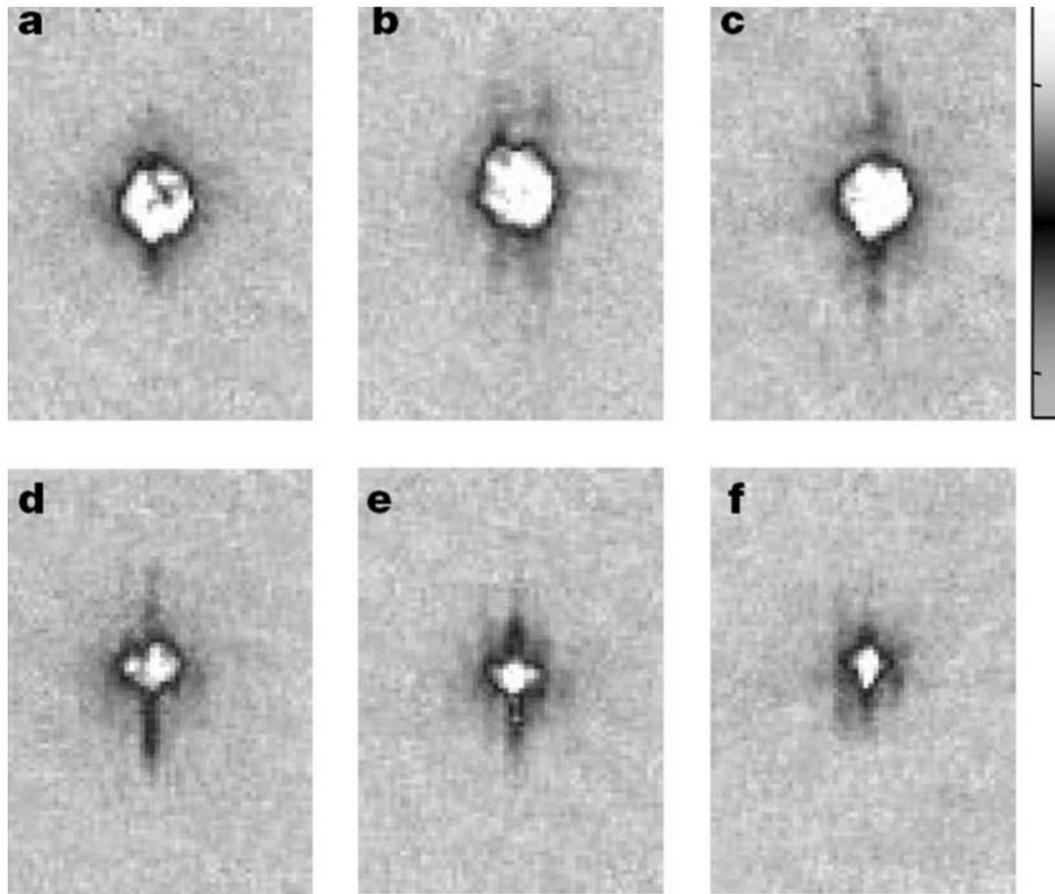
The Nobel Prize in Physics 2001 was awarded jointly to Eric A. Cornell, Wolfgang Ketterle and Carl E. Wieman "for the achievement of Bose-Einstein condensation in dilute gases of alkali atoms, and for early fundamental studies of the properties of the condensates." The main experimental results about observation of condensation were published in 1995. Such condensates are very interesting nonlinear objects which are very familiar to those in nonlinear optics. Their dynamics in the leading order with respect to the gas parameter can be described by the Gross-Pitaevskii equation (GPE) in the external potential modeling magnetic-optical traps. In nonlinear optics and plasma physics this equation after simple rescaling coincides with NLSE.

Introduction: history and experimental data

- As well known from quantum mechanics, the scattering amplitude f_l with angular momentum l behaves at small k proportionally to k^l . Therefore at low temperature $T \rightarrow 0$ interaction between cold atoms is connected with s-scattering, characterized by the s-wave scattering length a_s . If $a_s > 0$ atoms are repelled, in the opposite case we have attraction between atoms. In the first case due to both repulsion and magnetic trap dynamics of condensate is stable. Attraction between atoms leads to the instability of the condensate and to forthcoming collapse. In nonlinear optics this instability is known as modulation instability. In the first experiments for Bose atoms $a_s > 0$ and therefore nothing extraordinary was not observed in the condensate dynamics.

Introduction: history and experimental data

The first experiments with negative a_s were performed with ^{85}Rb by Donley et al., 2001 (below) and Roberts et al., 2001.



Introduction: history and experimental data

- Study of collapse of the gaseous Bose-Einstein condensates (BECs) became possible due to using the Fano-Feschbach resonance technique when the scattering lengths a_s can be effectively changed from positive to negative values. Initially in the experiments there was used the regime of positive a_s that results in formation of stable condensate. Then the a_s is increased and becomes negative. This leads to instability and forthcoming collapse when small "singular" regions with high atomic density are formed. Development of collapse, as was shown in many experiments, is accompanied by escape of almost all atoms from the magnetic traps (more than 50 %). Therefore it was necessary to explain these experimental facts.

Introduction: history and experimental data

- The first explanation was given by Yu.M. Kagan with co-authors in 1997. They suggested the mechanism based on recombination of three atoms with the formation of dimer (like H_2) and one atom carrying out the momentum access.
- When the mean distance between atoms $\sim n^{-1/3}$ much larger the scattering length a_s then, in the leading order relative to small gas parameter $na_s^3 \ll 1$, for temperatures $T \rightarrow 0$, the condensate dynamics can be described within the Gross-Pitaevskii (GP) approximation,

$$\hat{H} = \int d\mathbf{r} \left[\hat{\psi}^\dagger(\mathbf{r}) \hat{H}_0 \hat{\psi}(\mathbf{r}) + \frac{U_0}{2} \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}(\mathbf{r}) \hat{\psi}(\mathbf{r}) \right].$$

Introduction: history and experimental data

- Here $\hat{H}_0 = -\frac{1}{2}\nabla^2 + V_0(\mathbf{r})$ is the one-particle Hamiltonian in the anisotropic oscillatory trap with

$$V_0(\mathbf{r}) = \frac{1}{2}(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2)$$

with frequencies $\omega_x, \omega_y, \omega_z$. We use units for which fundamental constants are equal unity: $\hbar = m = 1$.

- For ultra-cold atoms, as known, main contribution to scattering comes from the s-scattering that allows to take the interaction potential $U(\mathbf{r})$ in the form

$U(\mathbf{r}) = U_0\delta(\mathbf{r})$. The scattering length is defined as

$U_0 = 2\pi a_s$ (in dimensional units $U_0 = 2\pi\hbar^2 a_s/m$).

Positive a_s corresponds to repulsion between atoms gas and $a_s < 0$ to attraction. Note that according to the 1st Born approximation the scattering amplitude

$f = -\frac{2m}{\hbar^2} \int U(r)e^{i\mathbf{q}\mathbf{r}} d\mathbf{r}$. Hence at $k \rightarrow 0$ we have $f = -a_s$.

Introduction: history and experimental data

- In the collapse regime we can ignore influence of trap and arrive at the standard quantum NLSE with $V_0 = 0$.
- Hence by decomposition of $\hat{\psi}$,
$$\hat{\psi} = \phi + \hat{\chi},$$
we give the condensate wave function (*c*-number) $\phi = \langle \hat{\psi} \rangle$ and the operator $\hat{\chi}$, responsible for the non-condensate atoms, has zero expectation value, $\langle \hat{\chi} \rangle = 0$.
- For small density of the non-condensate atoms ϕ satisfies the GPE (which coincides with the NLSE),

$$i\phi_t + \frac{1}{2}\Delta\phi + |\phi|^2\phi = 0,$$

Introduction: history and experimental data

- It follows immediately that the three-body recombination, as inelastic process, appears in the next order relative to na_s^3 . As the result, the GPE gets additional term $iK_3|\phi|^4\phi$ with constant $K_3 > 0$:

$$i\phi_t + \frac{1}{2}\Delta\phi + |\phi|^2\phi + iK_3|\phi|^4\phi = 0.$$

- In nonlinear optics this term is responsible for multi-photon absorption.

Main goals

- In this paper we suggest a new mechanism within the Gross-Pitaevskii approximation (GPA) which does not contain additional small gas parameter. It is connected with generation of non-condensate particles due to the coherence destruction of collapsing condensate. We show that the generation of non-condensate particles in the framework of the GPA (this is a quantum problem) for small density of non-condensate particles reduces to the linear problem for the normal and anomalous correlators:

$$\begin{aligned}n(\mathbf{x}, \mathbf{x}', t) &= \langle \hat{\chi}^\dagger(\mathbf{x}, t) \hat{\chi}(\mathbf{x}', t) \rangle, \\ \sigma(\mathbf{x}, \mathbf{x}', t) &= \langle \hat{\chi}(\mathbf{x}, t) \hat{\chi}(\mathbf{x}', t) \rangle.\end{aligned}$$

Main goals

- These correlators due to inhomogeneous background depend on both time and two coordinates \mathbf{r}_1 and \mathbf{r}_2 , but not on their difference as in the case of homogeneous background. The normal correlator at $\mathbf{r}_1 = \mathbf{r}_2$ represents density of non-condensate particles n and the anomalous correlator σ (at $\mathbf{r}_1 = \mathbf{r}_2$) is responsible for particle exchange between condensate and non-condensate reservoirs:

$$\partial_t \int n(\mathbf{r}) d\mathbf{r} = -2 \int \text{Im}[\phi^2 \sigma^*] d\mathbf{r} = -\partial_t \int |\phi|^2 d\mathbf{r}.$$

Just the anomalous correlator describes the coherence "transfer" from condensate to non-condensate particles. Note that between normal and anomalous correlators there exists the following inequality: $n \geq |\sigma|$.

Historical remark

- The anomalous correlators in physics appeared in the Bardeen-Cooper-Schrieffer (BCS) theory of superconductivity where the correlators are responsible for pairing of two electrons with opposite directions of spins (1957).
- In nonlinear wave physics such type of correlators were introduced in the so-called S-theory by Zakharov, Lvov and Starobinets (Sov. Phys. Uspekhi, 17(6), 896-919, (1975)). S-theory describes the parametric excitation of spin waves in ferromagnetics due to monochromatic electromagnetic wave. This σ -correlator is responsible for transition of coherence from the monochromatic wave to spin waves. If $\sigma = 0$ then excitation is impossible. Unlike our case the σ -correlators for spin waves in the S-theory depend on the difference $\mathbf{r}_1 - \mathbf{r}_2$.

Main goals

- The equations of motion for correlators are obtained in the framework of the Hartree-Fock-Bogolyubov (HFB) approximation.
- For small density of non-condensate particles the equations for $n(x, x')$ and $\sigma(x, x')$ are linear:
- $$i\partial_t n(x', x) = -\frac{1}{2}(\Delta - \Delta')n(x', x) + 2n(x', x)(|\phi|^2 - |\phi'|^2) + \phi^2\sigma^*(x', x) - \phi'^2\sigma(x', x),$$
- $$i\partial_t \sigma(x', x) = -\frac{1}{2}(\Delta + \Delta')\sigma(x', x) + 2\sigma(x', x)(|\phi|^2 + |\phi'|^2) + \phi^2 n(x, x') + \phi'^2 n(x', x),$$
 where prime means dependence on x' .
- In this case these linear equations for correlators admit separation of variables that leads to the linearized GP equation on the background of the collapsing solution.

Main goals

- Hence, the quantum problem about the non-condensate particles generation reduces to the linear stability analysis for collapsing regime, describing by the GPE. As it was shown by Zakharov and Kuznetsov (1986), in the 3D NLSE there are a few possible regimes of collapses: quasi-classical strong collapse when a finite amount of particles is captured into singularity, quasi-classical weak collapses when formally zeroth amount of particles can be captured into singularity and a weak collapse describing by the self-similar solution of the NLSE.
- Quasi-classical approximation corresponds to the Thomas-Fermi approach. In Zakharov-Kuznetsov paper it was shown that all quasi-classical regime of collapses are unstable except probably the only one, i.e., the weak collapse.

Strong collapse

Make a few general remarks.

- The GPE describes for particle motion in the self-consistent potential $V = V_0(\mathbf{r}) - |\phi|^2$. For small gas density ϕ is defined mainly by the trap. However, increase in density opens the so-called modulation instability with the growth rate $\gamma = k(|A|^2 - k^2/4)^{1/2}$ (A is the condensate amplitude) which appears due to attraction and saturates at $k_{cr} = 2|A|$.
- For $k_{cr} \gg \lambda^{-1}$ influence of the trap to the modulation instability can be neglected where $\lambda \sim \omega^{-1/2}$ is the trap ground state size. It gives $n_0 \gg n_{cr} \sim (\omega)^{-1}$.

Strong collapse

- In the opposite case, the trap influence is more essential but even in this case we have only quasi-stationary state. It follows from the scaling transformation remaining $\varphi(\mathbf{r}) \rightarrow \alpha^{-3/2}\varphi(\mathbf{r}/\alpha)$ remaining the total N . Under this transform the Hamiltonian becomes function of the scaling parameter α

$$H(\alpha) = \frac{\omega^2 \alpha^2}{2} I_r + \frac{1}{2\alpha^2} I_1 - \frac{1}{2\alpha^3} I_2$$

where

$$I_r = \int r^2 |\varphi|^2 d\mathbf{r}, \quad I_1 = \int |\nabla \varphi|^2 d\mathbf{r}, \quad I_2 = \int |\varphi|^4 d\mathbf{r}.$$

- $H(\alpha)$ tends to $-\infty$ as $\alpha \rightarrow 0$ independently on the first two terms.

Strong collapse

- Thus, H is unbounded functional that is one of the main criteria of collapse in this system. Collapse in this case can be considered as particle falling down in the unbounded self-consistent potential. At small number of $N_0 \lesssim N_{cr}$, H has a local minimum due to the trap. However, a state corresponding to this minimum will be always quasi-stationary. The latter means that particles which were initially in this state will tunnel through the barrier and collapse afterwards. Of course, in this case the total number of particles must be macroscopically large.
- The Hamiltonian unboundedness can be established also for arbitrary (but finite) values of ω_i . Thus, the system must evolve to the collapse regime for any initial (but macroscopically large) conditions. Sufficient criterion of collapse is $H < 0$, according to the virial theorem.

Strong collapse: solution

- The GPE in the Thomas-Fermi approximation is written for density n_0 and phase Φ_0 as

$$\partial_t n_0 + \text{div}(n_0 \nabla \Phi_0) = 0,$$

$$\partial_t \Phi_0 + \frac{(\nabla \Phi_0)^2}{2} - n_0 = 0.$$

- According to Zakharov and Kuznetsov (1986), the exact spherically symmetric collapsing solution of these Eqs. has the form:

$$n_0(\mathbf{r}, t) = a^{-3}(t) \lambda^2 (1 - \xi^2)$$

where

$$\xi = r/a(t), \quad \Phi_0(\xi, t) = \frac{1}{2} a(t) \dot{a}(t) \xi^2 + \tilde{\Phi}_0(t).$$

Strong collapse: solution

- For this solution $\lambda = \sqrt{3N_0/\pi}$ and the radial scaling parameter $a(t)$ satisfies Newton equation $\ddot{a}(t) = -\frac{\partial V}{\partial a}$ that describes the falling of a classical particle to the center in the potential $V = -2\lambda^2/(3a^3)$.
- Asymptotically a tends to the power dependence: $a(t) \rightarrow (5/\sqrt{3})^{2/5} (t_0 - t)^{2/5}$ and $n_0 \sim (t_0 - t)^{-6/5}$.
- This solution is meaningful only at $\xi \leq 1$, and if $\xi > 1$ n_0 is set equal to zero.
- Point $\xi = 1$ for this solution plays the same role as the turning point for the 1D stationary Schrodinger equation. This means the found solution should be matched with the linear solution at $\xi > 1$. It is interesting that the matching area $\Delta\xi$ in this case vanishes like

$$a^{1/3} \lambda^{-2/3}$$

Strong collapse: instability

- Linear stability analysis shows (see ZK, 1986) instability of the constructed exact semi-classical solution.
- Since $|\phi|^2 > 1/a^2$ for a strong collapse, the most dangerous from the standpoint of stability are shortwave perturbations with $k \gg 1/a$. Recall that the growth rate of the modulation instability $\Gamma = \sqrt{k^2 A^2 - k^4/4}$ has a maximum at $k = 2A$ when the dispersion terms in the maximum region are of the order of the nonlinear ones. Thus at $k^2 \ll |A|^2$ the dispersion terms, conversely, are insignificant and the instability is quasiclassical in this case.
- Because of shrinking the collapsing region, it is evident that the wave number changes in time as $k = p/a(t)$ where p is a time independent number and $A^2 = \lambda^2/a^3$.

Strong collapse: instability

- Thus, the time dependent growth rate $\Gamma(t) \approx \sqrt{\lambda^2 p^2 / a^5} \rightarrow \frac{3}{25} p (t_0 - t)^{-1}$. Hence by integrating of this expression in time we get how the perturbation behaves in time: $\exp\left(\int \Gamma(t) dt\right) \rightarrow (t_0 - t)^\gamma$ where $\gamma = -\sqrt{3}p/5$. Since $p \gg 1$ this means the instability of the strong-collapse regime relative to short-wave perturbations.
- Exact analysis of the linearized problem confirms this result.

Anisotropic collapse

- In the anisotropic case, collapsing semi-classical solutions of GPE can be found by the same procedure as in the isotropic case

$$n_0(\mathbf{r}, t) = \frac{1}{b_x(t)b_y(t)b_z(t)} f_0 \left(\xi = \frac{x}{b_x(t)}, \eta = \frac{y}{b_y(t)}, \zeta = \frac{z}{b_z(t)} \right).$$

The continuity equation is also integrated explicitly. The eikonal equation gives $f_0 = \lambda^2(1 - \xi^2 - \eta^2 - \zeta^2)$ where $b_i(t)$ are defined from coupled Newton equations,

$$\ddot{b}_i = 2 \frac{\lambda^2}{b_i b_x b_y b_z},$$

with the potential $V = -2\lambda^2(b_x b_y b_z)^{-1}$.

Anisotropic collapse

- In the axial-symmetrical case, we have two equations for $b_x = b_y$ and b_z . Their analysis shows two kind behaviors:

$$b_x(t) \rightarrow 2\lambda \sqrt{\frac{|U_0|}{b_z(t_0)}} \sqrt{t_0 - t}, \quad b_z(t) \rightarrow b_z(t_0)$$

with collapse to sigar-shape form;

$$b_x(t) \rightarrow b_x(t_0), \quad b_z(t) \rightarrow \left(\frac{9|U_0|\lambda^2}{b_x^2(t_0)} \right)^{1/3} (t_0 - t)^{2/3}$$

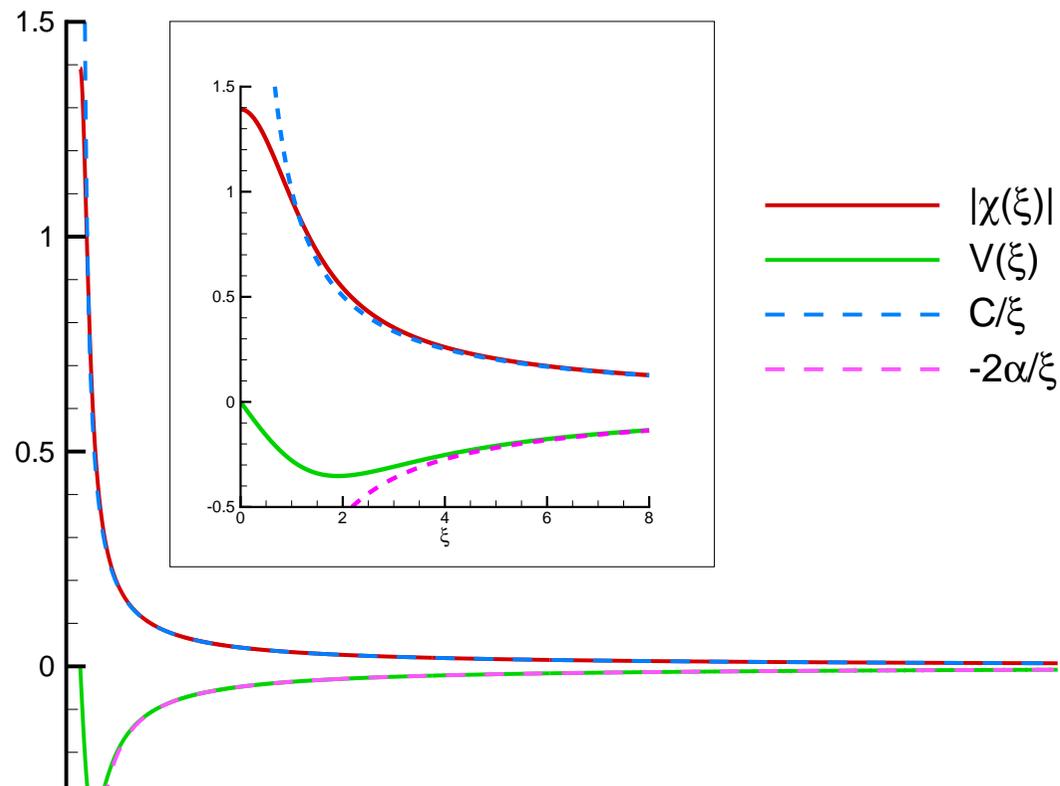
with collapse into disk-shape form. Such types of collapses were observed in JILA experiment with formation of thorns (Donley, et al, Nature, 2001). The authors used instead of «thorns» the word «jets».

Weak semi-classical collapses

- Besides the strong collapse solution the GPE in the semi-classical limit has also the whole family of self-similar solutions with amplitude $A \sim (t_0 - t)^{-\beta}$ and scale $a \sim (t_0 - t)^{1-\beta/2}$ for which $6/5 > \beta > 1$. It is possible to check by means of the same argumentation that all of them are also unstable. In this case $\beta = 6/5$ corresponds to the strong collapse regime, and $\beta = 1$ to weak collapse.

Weak collapse

- Weak collapse is described by the self-similar solution of the GPE: $\psi = (t_0 - t)^{-1/2 - i\alpha} \chi \left[\frac{|\mathbf{r} - \mathbf{r}_0|}{(t_0 - t)^{1/2}} \right]$ where $\alpha = 0.545$, at $\xi \rightarrow \infty$ $\chi \rightarrow \frac{C}{\xi^{1+2i\alpha}}$ with $C = 1.01$.
 $V = \arg(\chi_\xi)$



Weak collapse

- Linearization of the GPE on the background of the self-similar solution, $\chi \rightarrow \chi + u$, gives for perturbation u

$$i \frac{\partial u}{\partial \tau} + i(1/2 + i\alpha)u + \frac{i}{2}\xi u' + \frac{1}{2}\Delta u + 2|\chi|^2 u + \chi^2 u^* = 0, \text{ C.C.Eq.}$$

where

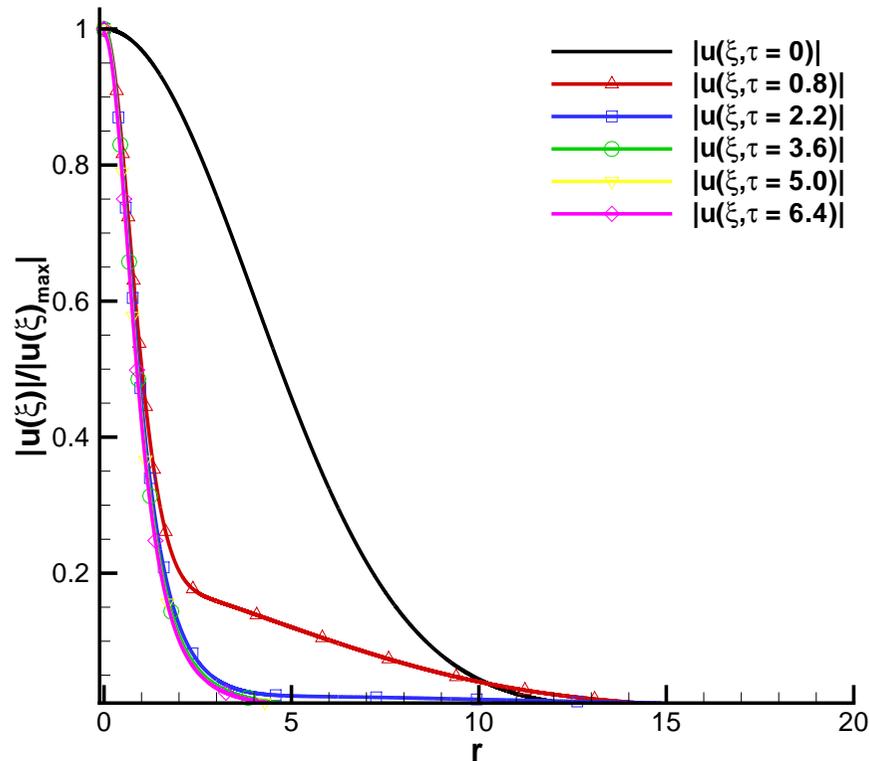
$$\Delta = \frac{1}{\xi^2} \frac{\partial}{\partial \xi} \xi^2 \frac{\partial}{\partial \xi} - \frac{l(l+1)}{\xi^2}$$

and $\tau = -\ln \frac{t_0 - t}{t_0}$ is the new «logarithmic» time.

- These equations were solved numerically with initial condition in the Gaussian form, multiplied by ξ^l , for different l . The mode $l = 0$ was most unstable. It grows exponentially $\sim \exp(\gamma_{max}\tau)$ as $\tau \rightarrow \infty$ with the growth rate $\gamma_{max} = 0.984984$.

Weak collapse

- The most unstable mode $l = 0$ has the form:



- All other perturbations with $l \geq 2$ occur stable.

Weak collapse

- It is worth noting that the recent experimental observations (Phys. Rev. X **6**, 041058 (2016)) show that collapses in gaseous BECs with low densities should be related to the weak collapse regimes.
- From another side after these numerics we could say that we have found instability of weak collapse that should provide generation of non-condensate atoms. However, γ_{max} in numerics was very close to unity. We know if any nonlinear solution depends on some parameters, derivative of such solution relative to the parameters satisfies the linearized equation. Differentiation ψ_s against t_0 gives exactly the growth rate $\gamma = 1$. Then we have checked that the obtained in numerics unstable mode coincides exactly with this shift mode and can not provide instability. Note that first time such shift mode was exploited by Barenblatt and Zel'dovich for flame wave (1965).

Weak collapse

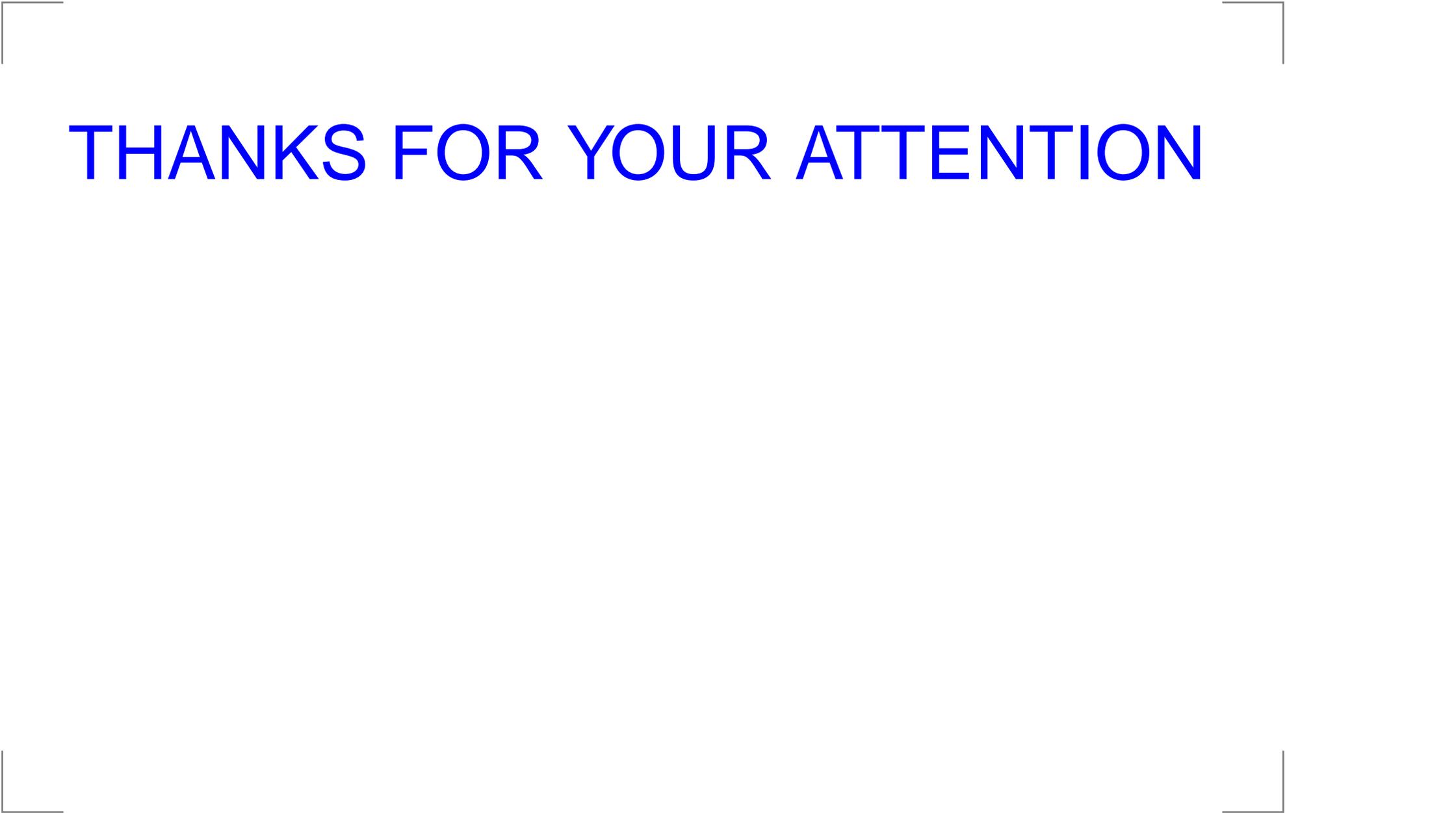
- Thus, in the Thomas-Fermi regime, we immediately arrive at the generation of non-condensate particles. As for the stability of a weak collapse and, accordingly, the formation of non-condensate particles in the weak collapse, this problem remains open up to now.
- Also note that the first numerical simulations (Zakharov, Kuznetsov, Musher, 1984) demonstrated that collapse in the 3D NLSE has the behavior corresponding to a weak collapse.
- Mention also papers (Vlasov, Piskunova and Talanov, 1984) and (Zakharov et al. 1989) where it was found the so-called black holes regime resulting in appearance of logarithmic corrections to $1/r^2$ -singularity for density.
- In the paper by V. Malkin and E. Shapiro (JETP, 1989) there was some numerical indication to instability of weak collapse.

Conclusion

- We suggest a new mechanism of the collapse destruction for gaseous Bose-Einstein condensates (BECs) with attraction connected with loss of the condensate coherence and generation of the non-condensate particles. This process is described within the Gross-Pitaevskii (GP) approximation.
- We derive the corresponding equations for the normal and anomalous pair correlators characterizing the non-condensate atom component for smaller non-condensate number density in comparison with the condensate density. The normal correlator depending on coordinates \mathbf{x} and \mathbf{x}' and on time t as well represents at $\mathbf{x} = \mathbf{x}'$ a density of the non-condensate atoms, the anomalous correlator is responsible for atom exchange between the condensate and non-condensate components.

Conclusion

- We show that the generation of non-condensate atoms is possible if the collapsing solution of the GP equation will be linearly unstable.
- Within the time-dependent Thomas-Fermi (TF) approximation we analyze the linear stability problem of the semi-classical collapsing solution found by Zakharov and Kuznetsov (1986).



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