

Collapse and stable self-trapping for Bose-Einstein condensates with $1/r^b$ type attractive interatomic interaction potential

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(Dated: February 7, 2010)

We consider dynamics of Bose-Einstein condensates with long-range attractive interaction proportional to $1/r^b$ and arbitrary angular dependence. It is shown exactly that collapse of Bose-Einstein condensate without contact interactions is possible only for $b \geq 2$. Case $b = 2$ is critical and requires number of particles to exceed critical value to allow collapse. Critical collapse in that case is strong one trapping into collapsing region a finite number of particles. Case $b > 2$ is supercritical with expected weak collapse which traps rapidly decreasing number of particles during approach to collapse. For $b < 2$ singularity at $r = 0$ is not strong enough to allow collapse but attractive $1/r^b$ interaction admits stable self-trapping even in absence of external trapping potential.

PACS numbers: 03.75.Kk, 03.75.Lm

The dynamics of Bose-Einstein condensate (BEC) with short-range s-wave interaction have been the subject of extensive research in recent years [1, 2]. Condensates with a positive scattering length have a repulsive (defocusing) nonlinearity which stabilizes the condensate with the help of external trap. Condensates with a negative scattering length have an attractive (focusing) nonlinearity which formally admits solitons. However, without trap these solitons are unstable and their perturbation leads either to collapse of condensate or condensate expansion. External trap prevents expansion of condensate and makes solitons metastable for a sufficiently small number of atoms. Otherwise, for larger number of atoms, the focusing nonlinearity results in collapse of solitons. The effect of a long-range dipolar interaction on BEC was first studied theoretically [3–7] and more recently observed experimentally [8–10] (see also [11, 12] for review). In particular, collapse of BEC with dominant dipole-dipole forces predicted based on approximate variational estimate [5] and obtained based on exact analysis [6] was recently observed in experiment [13].

Here we look for possibility of collapse of BEC due to long-range attraction vs. formation of stable self-trapped condensate for a general type of long-range interaction

$$V(\mathbf{r}) = \frac{f(\mathbf{n})}{r^b}, \quad b > 0, \quad \mathbf{n} \equiv \frac{\mathbf{r}}{r}, \quad r \equiv |\mathbf{r}|, \quad (1)$$

where $f(\mathbf{n})$ is an arbitrary bounded function $|f(\mathbf{n})| < \infty$ and $\mathbf{r} = (x_1, x_2, x_3)$. We do not require $f(\mathbf{n})$ to be sign-definite. By attractive interaction we mean that $f(\mathbf{n})$ is negative at least for some nonzero range of angles so that one can choose a wave function to provide negative contribution to energy functional.

Possible experimental realization of (1) are numerous. E.g., recent experimental advances allow to study interaction of ultracold Rydberg atoms with principle quantum number about 100 (see e.g. [14, 15]). These interactions between atoms in highly excited Rydberg levels are long-range and dominated by dipole-dipole-type forces.

Strength of interaction between Rb atoms is about 10^{12} times stronger (at typical distance $\sim 10\mu\text{m}$) than interaction between Rb atoms in ground state (see e.g. [15] for review). Strength and angular dependence of interaction between Rydberg atoms can be tuned in a wide range [15, 16]. E.g., spatial dependence for Rb with principle quantum number about 100 can be $\propto 1/r^3$ for $r \lesssim 9.5\mu\text{m}$ and $\propto 1/r^6$ (van der Waals character) for $r \gtrsim 9.5\mu\text{m}$ [15]. Short-range s-wave scattering interaction is limited to much smaller distance \sim few nm so that the range of dominance of long-range interaction potential is quite high. Another possible form of long-range attractive interaction is gravity-like $1/r$ potential which is proposed to be realized in a system of atoms with laser induced dipoles such that an arrangement of several laser fields causes cancelation of anisotropic terms [17]. Terms $\propto 1/r^2$ are also possible [17].

The mean field BEC dynamics is governed by a nonlocal Gross-Pitaevskii equation (NGPE)

$$i\hbar \frac{\partial \Psi(\mathbf{r})}{\partial t} = \left[-\frac{\hbar^2}{2m} \nabla^2 + \frac{1}{2} m \omega_0^2 (x_1^2 + x_2^2 + \gamma^2 x_3^2) + g |\Psi(\mathbf{r})|^2 + \int d^3 \mathbf{r}' V(\mathbf{r} - \mathbf{r}') |\Psi(\mathbf{r}')|^2 \right] \Psi(\mathbf{r}), \quad (2)$$

where Ψ is the condensate wave function, the contact interaction is $\propto g = 4\pi\hbar^2 a/m$, a is the s-wave scattering length, m is the atomic mass, ω_0 is the external trap frequency in the $x_1 - x_2$ plane, γ is the anisotropy factor of the trap, and the wavefunction is normalized to the number of atoms, $\int d^3 \mathbf{r} |\Psi|^2 = N$. Contact interaction term can be also included into potential $V(\mathbf{r})$ as $\frac{g}{2} \delta(\mathbf{r})$ but we have not done that because we focus here on effect of long-range potential (1). If $V(\mathbf{r}) \equiv 0$ then a standard Gross-Pitaevskii equation (GPE) [1] is recovered.

NGPE (2) can be written through variation $i\hbar \frac{\partial \Psi}{\partial t} = \frac{\delta E}{\delta \Psi^*}$ of the energy functional

$$E = E_K + E_P + E_{NL} + E_R, \quad (3)$$

which is an integral of motion: $\frac{dE}{dt} = 0$, and

$$\begin{aligned} E_K &= \int \frac{\hbar^2}{2m} |\nabla\Psi|^2 d^3\mathbf{r}, & E_{NL} &= \frac{g}{2} \int |\Psi|^4 d^3\mathbf{r}, \\ E_P &= \int \frac{1}{2} m\omega_0^2 (x_1^2 + x_2^2 + \gamma^2 x_3^2) |\Psi|^2 d^3\mathbf{r}, & (4) \\ E_R &= \frac{1}{2} \int |\Psi(\mathbf{r})|^2 V(\mathbf{r} - \mathbf{r}') |\Psi(\mathbf{r}')|^2 d^3\mathbf{r} d^3\mathbf{r}'. \end{aligned}$$

Consider time evolution of the mean square radius of the wave function, $\langle r^2 \rangle \equiv \int r^2 |\Psi|^2 d^3\mathbf{r} / N$. Using (2), integrating by parts, and taking into account vanishing boundary conditions at infinity one obtains

$$\partial_t \langle r^2 \rangle = \frac{\hbar}{2mN} \int 2ix_j (\Psi \partial_{x_j} \Psi^* - \Psi^* \partial_{x_j} \Psi) d^3\mathbf{r}, \quad (5)$$

where $\partial_t \equiv \frac{\partial}{\partial t}$, $\partial_{x_j} \equiv \frac{\partial}{\partial x_j}$ and repeated index j means summation over all space coordinates, $j = 1, \dots, 3$. After a second differentiation over t , one gets [6]

$$\begin{aligned} \partial_t^2 \langle r^2 \rangle &= \frac{1}{2mN} \left[8E_K - 8E_P + 12E_{NL} \right. \\ &\quad \left. - 2 \int |\Psi(\mathbf{r})|^2 |\Psi(\mathbf{r}')|^2 (x_j \partial_{x_j} + x'_j \partial_{x'_j}) V(\mathbf{r} - \mathbf{r}') d^3\mathbf{r} \right], \quad (6) \end{aligned}$$

which is called by a virial theorem [6] similar to GPE [18–23].

It follows from (1) that $(x_j \partial_{x_j} + x'_j \partial_{x'_j}) V(\mathbf{r} - \mathbf{r}') = -bV(\mathbf{r} - \mathbf{r}')$ and using (3) we rewrite (6) as follows

$$\begin{aligned} \partial_t^2 \langle r^2 \rangle &= \frac{1}{2mN} \left[4bE + (8 - 4b)E_K - (4 + 2b)m\omega_0^2 \langle r^2 \rangle \right. \\ &\quad \left. - (4 + 2b)m\omega_0^2 N(\gamma^2 - 1) \langle x_3^2 \rangle + (12 - 4b)E_{NL} \right]. \quad (7) \end{aligned}$$

Here both the local nonlinear term E_{NL} and the nonlocal nonlinear term E_R are included into the energy E . Catastrophic collapse of BEC in terms of NGPE means a singularity formation, $\max |\Psi| \rightarrow \infty$, in a finite time. Because of conservation of N , the typical size of atomic cloud near singularity must vanish. The virial theorem (7) describes collapse when the positive-definite quantity $\langle r^2 \rangle$ becomes negative in finite time implying $\max |\Psi| \rightarrow \infty$ before $\langle r^2 \rangle$ turns negative. The kinetic energy E_K diverges at collapse time which follows from divergence of the potential energy for $\max |\Psi| \rightarrow \infty$ together with conservation of the energy functional E . Another way to see divergence of E_K is from uncertainty relation $E_K \geq \frac{\hbar^2}{2m} (9/4) N / \langle r^2 \rangle$ (see [6, 20]) for $\langle r^2 \rangle \rightarrow 0$. Generally $\langle r^2 \rangle$ may not vanish at collapse (e.g. if there are nonzero values of $|\Psi|$ away from collapse center) but E_K diverges at collapse time for sure because of $\max |\Psi| \rightarrow \infty$. We use below divergence of E_K as necessary and sufficient condition of collapse formation while vanishing of $\langle r^2 \rangle$ is only sufficient condition for collapse.

NGPE is not applicable near singularity and another physical mechanisms are important such as inelastic two-

and three-body collisions which can cause a loss of atoms from the condensate [1]. In addition, multipole expansion used for derivation of the dipole-dipole-type potential is not applicable on a very short distances (few a few Bohr radii). However, as explained above, NGPE with potential (1) is a good approximation for a wide range of typical interatomic distances.

Consider case $2 \leq b \leq 3$. Then one immediately obtains from equation (7) that $\partial_t^2 \langle r^2 \rangle \leq \frac{6E}{mN}$. Integrating that differential inequality over time we get that $\langle r^2 \rangle \leq \frac{3E}{mN} t^2 + \partial_t \langle r^2 \rangle|_{t=0} t + \langle r^2 \rangle|_{t=0}$. If $E < 0$ we conclude that $\langle r^2 \rangle \rightarrow 0$ for large enough t which provides a sufficient criterion of collapse of BEC. Condition $E < 0$ is sufficient but not necessary for collapse. Using generalized uncertainty relations between E_K , N , $\langle r^2 \rangle$, $\partial_t \langle r^2 \rangle$ [6, 20] one can obtain much stricter condition of collapse which is outside the scope of this Letter.

Below we assume $g = 0$. Choosing e.g. initial condition as $\psi|_{t=0} = \frac{N^{1/2}}{\pi^{3/4} r_0^{3/2}} e^{-r^2/(2r_0^2)}$ gives $E = -\frac{3\hbar^2 N}{4m r_0^2} + \pi^{-1/2} 2^{4-b} f N^2 r_0^{-b} \Gamma(3/2 - b/2)$ for $\omega_0 = 0$ and $f(\mathbf{n}) = \text{Const} \equiv f$. If the constant r_0 is small and $b > 2$ or if $N > 3\hbar^2/(16mf)$ and $b = 2$ then $E < 0$. It means that for $2 \leq b \leq 3$ long-distance potential alone is enough to achieve catastrophic collapse of BEC. Another particular example was considered in Ref. [6] for the case of dipole-dipole interaction potential with all dipoles oriented in one fixed direction. Note also that $b = 3$ is a border between short-range potentials (for $b > 3$) and long-range potentials (for $b \leq 3$) in 3D (one needs convergence of $\int_{r < r_c} V(\mathbf{r}) d^3\mathbf{r}$ to have short-range potential, where r_c is a cutoff at small distances). Case $b = 3$ also requires that integral of $V(\mathbf{r})$ over angles to be zero to ensure convergence of (1) at small r (as is the case [6] for dipole-dipole interactions with fixed direction) otherwise we would have to introduce cutoff at small distances and potential would lose general form (1).

Case $b > 3$ generally requires introduction of cutoff at small scales. Because $\int_{r < r_c} V(\mathbf{r}) d^3\mathbf{r}$ is finite in that case we generally have situation very similar to standard δ -correlated potential [1].

Now we prove that for $b < 2$ collapse is impossible for $g = 0$ because singularity of (1) is not strong enough. We use the inequality $\int \frac{|\Psi(\mathbf{r})|^2}{|\mathbf{r} - \mathbf{r}'|^2} d^3\mathbf{r} \leq 4 \int |\nabla\Psi(\mathbf{r})|^2 d^3\mathbf{r}$ [24], which holds for any \mathbf{r}' . Using now Hölder's inequality we generalize that inequality (assuming $b < 2$) as follows

$$\begin{aligned} &\int \frac{|\Psi(\mathbf{r})|^2}{|\mathbf{r} - \mathbf{r}'|^b} d^3\mathbf{r} = \int |\Psi(\mathbf{r})|^{2-b} \frac{|\Psi(\mathbf{r})|^b}{|\mathbf{r} - \mathbf{r}'|^b} d^3\mathbf{r} \\ &\leq \left[\int (|\Psi(\mathbf{r})|^{2-b})^{\frac{1}{1-b/2}} d^3\mathbf{r} \right]^{1-\frac{b}{2}} \\ &\times \left[\int \left(\frac{|\Psi(\mathbf{r})|^b}{|\mathbf{r} - \mathbf{r}'|^b} \right)^{\frac{2}{b}} d^3\mathbf{r} \right]^{\frac{b}{2}} \leq 2^b N^{1-\frac{b}{2}} \left(\frac{2m}{\hbar^2} E_K \right)^{\frac{b}{2}}. \quad (8) \end{aligned}$$

Using now boundness of f : $f(\mathbf{n}) \leq f_m \equiv \max_{\mathbf{n}} |f(\mathbf{n})|$ in

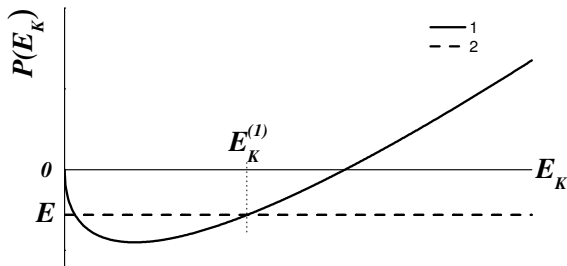


FIG. 1: Schematic of the function $P(E_K)$ defined in (10) (solid curve). Equation $P(E_K) = E$ (E corresponds to dashed line) has either one of two roots for $E_K > 0$ depending on sign of E . $E_K^{(1)}$ is the largest root.

(1) and inequality (8) we obtain a bound for E_R in (4)

$$E_R \geq -f_m 2^{b-1} N^{2-\frac{b}{2}} \left(\frac{2m}{\hbar^2} E_K \right)^{\frac{b}{2}}, \quad (9)$$

which gives a respective bound of E in (4) (recall that we assume $g = 0$):

$$E \geq E_K - f_m 2^{b-1} N^{2-\frac{b}{2}} \left(\frac{2m}{\hbar^2} E_K \right)^{\frac{b}{2}} \equiv P(E_K). \quad (10)$$

A function $P(E_K)$ in (10) has a minimum for $E_K \equiv E_K^{(0)} = 2^{-2} [f_m b]^{2/(2-b)} N^{\frac{4-b}{2-b}} (2m/\hbar^2)^{b/(2-b)}$ resulting in a lower bound

$$E \geq -\frac{2-b}{b} 2^{-2} [f_m b]^{\frac{2}{2-b}} N^{\frac{4-b}{2-b}} \left(\frac{2m}{\hbar^2} \right)^{\frac{b}{2-b}}. \quad (11)$$

Boundness of the energy functional E from below ensures that collapse is impossible for $b < 2$. To prove that we show that E_K is bounded while collapse requires $E_K \rightarrow \infty$. We choose any value of E which satisfy (11). Fig. 1 shows schematically the function $P(E_K)$ from (10). Inequality (10) requires that $E_K \leq E_K^{(1)}(E)$, where $E_K^{(1)}(E)$ is the largest root of equation $P(E_K) = E$. It proves that E_K is bounded for fixed N which completes the proof of absence of collapse for $b < 2$. Particular version of that result for $b = 1$ and $f(\mathbf{n}) = \text{const}$ was first obtained in Ref. [25]. Nonexistence of collapse for nonsingular potential $V(\mathbf{r})$ was shown previously based on approximate analysis in Ref. [26]. Proof of nonexistence of collapse for particular example of nonsingular potentials with positive-definite bounded Fourier transform was given in Ref. [27]. These results can be easily generalized for any bounded potential similar to above analysis. Thus collapse can occur for singular potential only and singularity should be strong enough, i.e. $b \geq 2$.

We now look for soliton solution of NGPE (2) as $\Psi(\mathbf{r}, t) = A(\mathbf{r})e^{-i\mu t/\hbar}$, where μ is the chemical potential. In that case NGPE (2) reduces to time-independent

equation

$$\left[-\mu - \frac{\hbar^2}{2m} \nabla^2 + \frac{1}{2} m \omega_0^2 (x_1^2 + x_2^2 + \gamma^2 x_3^2) + \int d^3 \mathbf{r}' V(\mathbf{r} - \mathbf{r}') A(\mathbf{r}')^2 \right] A(\mathbf{r}) = 0, \quad (12)$$

where we again assume $g = 0$ although generalization to $g \neq 0$ case is straightforward. Equation (12) is the stationary point of the energy functional E for a fixed number of particles: $\delta(E - \mu N) = 0$. Multiplying equation (12) by A and $x_j \partial_{x_j} A$ and integrating by parts one obtains using (1) and (3) that

$$E_{K,s} = -\mu N_s \frac{b}{4-b} + E_{P,s}, \quad E_{R,s} = \mu N_s \frac{2}{4-b}, \quad (13)$$

$$E_s = -\mu N_s \frac{b-2}{4-b} + 2E_{P,s},$$

where subscript "s" means values of all integrals on soliton solution. Especially simple and interesting is the case of self-trapping ($\omega_0 = 0$) when condensate is in steady state without any external trap. All integrals in that case depend on number of particles N_s only.

Assume radial symmetry $f(\mathbf{n}) = \text{Const} < 0$ in (1). Ground state soliton is determined from condition that $A(\mathbf{r})$ never crosses zero [28, 29]. To prove ground soliton stability we show that it realizes a minimum of the Hamiltonian for a fixed N_s . One can make inequality (8) sharper by minimizing a functional $\mathcal{F}(\Psi) \equiv N^{1-\frac{b}{2}} \left(\frac{2m}{\hbar^2} E_K \right)^{\frac{b}{2}} / \int \frac{|\Psi(\mathbf{r})|^2}{|\mathbf{r}-\mathbf{r}'|^b} d^3 \mathbf{r}$. That minimum is achieved at one of stationary points $\frac{\delta \mathcal{F}}{\delta \Psi^*} = 0$ and after simple rescaling one can see that these points corresponds to soliton solutions of the time-independent NGPE (12). Among these stationary points the minimum is achieved at ground state soliton $\Psi_{s,\text{ground}}$. It gives a bound $\mathcal{F}(\Psi) \geq \min \mathcal{F}(\Psi) = \mathcal{F}(\Psi_{s,\text{ground}})$ which is sharper than the inequality (8). Most important is that following analysis similar to equations (9)-(11) we obtain that for any Ψ

$$E \geq \min E = E_{s,\text{ground}}, \quad (14)$$

i.e. the ground state soliton solution attains the minimum of E for fixed N . It proves exactly the stability of soliton for $f(\mathbf{n}) = \text{Const}$. Similar ideas were used in a nonlinear Schrödinger equation [28, 29]. Ground state soliton was also found numerically for $b = 1$ [30].

For more general $f(\mathbf{n}) \neq \text{Const}$ minimum of E is still negative if $f(\mathbf{n})$ is negative for a nonzero range of values of \mathbf{n} . So in that case we expect that ground state soliton attains that minimum and, respectively is stable. If $f(\mathbf{n}) > 0$ for any \mathbf{n} then $\min E = 0$. It corresponds to unbounded spatial spreading of NGPE solution for any initial conditions. Self-trapping is impossible in that case and solitons are possible for $\omega_0 \neq 0$ only.

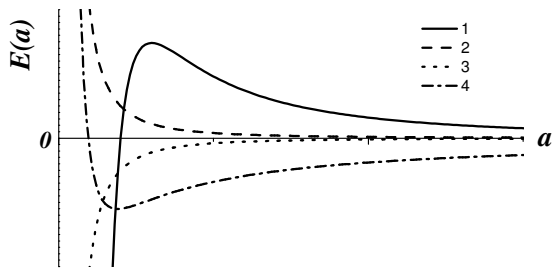


FIG. 2: Schematic of $E(a)$ from (15) for $b > 2$, $b = 2$ and $b < 2$ (see text for details).

Case $b = 2$ is on the boundary between bounded and unbounded energy functional as can be seen from inequalities (10) and (14). If $N > N_{s,ground}$ then E is unbounded. If $N < N_{s,ground}$ then $E \geq E_{s,ground} = 0$ as follows from (13) for $b = 2$. Thus $N_{s,ground}$ is the critical number of particles for collapse. That critical number is similar to collapse of GPE in dimension 2 (2D) (as well as similar to critical power in nonlinear optics) [18]. It is important to distinguish that critical number from the critical number of particles of 3D GPE with $\omega_0 \neq 0$ [1, 2].

To qualitatively distinguish different regimes of collapse and solitons one can consider, in addition to the exact analysis above, a scaling transformations [31] which conserves the number of particles $\Psi(\mathbf{r}) \rightarrow a^{-3/2}\Psi(\mathbf{r}/a)$. Under this transformation the energy functional E (for $\omega_0 = 0$) depends on the parameter a as follows

$$E(a) = a^{-2}E_K + a^{-b}E_R. \quad (15)$$

The virial theorem (7) and the relations (13), (15) have striking similarities with GPE if we replace b by the spatial dimension D in GPE. That analogy suggests to refer the case $b = 2$ as the critical NGPE and $b > 2$ as the supercritical NGPE. Fig. 2 shows typical dependence of (15) on a for $b > 2$, $b = 2$ and $b < 2$ assuming $E_R < 0$. For $b > 2$ there is a maximum of E (curve 1 in Fig. 2) corresponding to unstable soliton. Solution of NGPE either collapse or expand. For $b = 2$ there is no extremum and collapse is impossible for $N < N_{s,ground}$ (curve 2 in Fig. 2) while condensate can collapse for $N > N_{s,ground}$ (curve 3 in Fig. 2). Ground state soliton corresponds to $N = N_{s,ground}$ and $E = 0$ locating exactly at the boundary between collapsing and noncollapsing regimes. For $b < 2$ there is a minimum which corresponds to stable ground state soliton (curve 4 in Fig. 2).

Solutions of both GPE and NGPE with $\omega_0 = 0$ near collapse typically consist of background of nearly linear waves and a central collapsing self-similar nonlinear core. The scaling (15) describes the dynamics of the core with time-dependent a such that $a \rightarrow 0$ near collapse. Waves have negligible potential energy but carry

a positive kinetic energy $E_{waves} \simeq E_{K,waves}$. The total energy $E = E_{collapse} + E_{waves}$ is constant, where $E_{collapse}$ is the core energy. It follows from (15) that for $b = 2$ one can simultaneously allow conservation of N and $E_{collapse}$ so that negligible number of waves are emitted from the core. This scenario is called a strong collapse. If $b > 2$ then the term $\propto a^{-b}$ in (15) dominates with $E_{collapse} \rightarrow -\infty$ as $a \rightarrow 0$. Then the only way to ensure conservation of E is to assume strong emission of linear waves. Near collapse time only vanishing number of particles remains in a core (of course all that is true until NGPE loses its applicability) which is called weak collapse [31]. Strong collapse was shown to be unstable for supercritical GPE [31]. It suggests that collapse for $b > 2$ is of weak type.

Support was provided by NSF grant DMS 0807131.

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