Collapse of Bose-Einstein condensate with dipole-dipole interactions

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A dynamics of Bose-Einstein condensate of a gas of bosonic particles with long-range dipole-dipole interactions in a harmonic trap is studied. Sufficient analytical criteria are found both for catastrophic collapse of Bose-Einstein condensate and for long-time condensate existence. Analytical criteria are compared with variational analysis.

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Bose-Einstein condensation of dilute trapped atomic gases\[1, 2\] essentially depends on the interparticle interactions. In most experiments so far the dominated interactions were short-range van der Waals forces which are characterized by the $s$-wave scattering length $a$. Spatially homogeneous condensates with positive scattering length (repulsive interaction) are stable while condensates with negative scattering length (attractive interaction) are always unstable to local collapses\[3\] because the quantum pressure is absent in homogeneous condensates. The presence of trapping field allows to achieve a metastable Bose-Einstein condensate (BEC)\[3\] for $a < 0$ if the number of particles is small enough to ensure existence of local minima of energy functional\[3\].

Recent progress in creating of ultra-cold molecular clouds\[4, 5\] opens a new prospective for achieving BEC in a dilute gas of polar molecules and stimulates growing interest in study of BEC with dipole-dipole interactions\[6, 7, 8, 9, 10, 11, 12\]. Dipole-dipole forces are long-range and essentially anisotropic. Net contribution of dipole-dipole interactions can be either repulsive (positive dipole-dipole interaction energy) or attractive (negative dipole-dipole interaction energy) depending on the form of condensate cloud, its orientation relative to dipole polarization axes and trap geometry. Respectively stability and collapse of BEC strongly depends on clouds anisotropy which opens a whole bunch of new phenomena to be observed and makes task of achieving and control of BEC especially challenging.

Dipole-dipole interactions can dominate provided polar molecules are oriented by strong enough electric field. Similar effects can be achieved for ground-state atoms with electric dipole moments induced by a strong electric field\[13, 14\]. Another possible physical realization is atoms with laser induced electric dipole moments\[15\]. Dipole-dipole interactions can be also essential in BEC of atomic gas with large magnetic dipole moments\[16, 17\]. Magnetic interactions are usually dominated by van der Waals forces but effects of magnetic interactions can essentially amplified by reducing of scattering length $a$ via a Feshbach resonance\[18, 19\]. Analysis of this Letter can be applied for both cases of electric and magnetic dipole-dipole interactions.

In this letter sufficient analytical criteria are developed both for catastrophic collapse of BEC of a trapped gas of dipolar particles and for long-time condensate existence. Sufficient criteria allows to predict condensate collapse or, opposite, its long-time existence for given condensate energy, $E$, number of particles, $N$, initial mean square width of condensate, and initial kinetic energy of condensate. Analytical criteria are compared with results of variational approach\[20\], where collapse was predicted based on the absence of local minimum of ground state of energy functional provided number of condensate particle exceeds certain critical value. It is shown here that variational calculation gives threshold number of particles and condensate energy which are located between parameters regions where analytical criteria predict collapse and long-time condensate existence, respectively. It is proven in this Letter that collapse certainly occurs provided energy of the condensate exceeds a threshold value which is determined by the number of particles and trap parameters. Collapse of condensate is accompanied with dramatic contraction of the atomic cloud. Collapse is impossible provided number of particles and initial kinetic energy of condensate are below the critical values.

The time-dependent Gross-Pitaevskii equation (GPE) for atoms with long-range interactions and for a cylindrical harmonic trap is given by\[21\]:

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

where $\mathbf{r} = (x_1, x_2, x_3)$, $\Psi$ is the condensate wave function, coupling constant $g$ corresponds to short-range forces and is given by $g = 4\pi\hbar^2 a/m$, $a$ is the $s$-wave scattering length, $m$ is the atomic mass, $\omega_0$ is a trap frequency in $x_1 x_2$ plane, and $\gamma$ is the anisotropy factor of the trap. $\Psi(\mathbf{r}, t)$ is normalized to the total number of atoms in condensate: $N = \int |\Psi|^2 d^3 \mathbf{r}$. It is assumed that the system is away from shape resonances of $V(\mathbf{r})$\[20\] and that the long-range potential is due to the dipole-dipole interac-
tion, and is given by
\[ V(r - r') = \frac{[d_1(r) \cdot d_2(r')]}{|r - r'|^2} - 3 \frac{[d_1(r) \cdot u] [d_2(r') \cdot u]}{|r - r'|^2}, \]
where \( u = (r - r')/|r - r'| \). All the dipoles are assumed to point in the direction of trap axes (\( \hat{x}_3 \)-direction), i.e., \( d_1 = d_2 = dx_3 \). Potential with no dependence of \( d \) on \( r \) is a good approximation provided a typical interparticle distance exceeds a few Bohr radii.

GPE \( \text{(1)} \) can be also obtained from variation of energy functional, \( E : i\hbar \frac{d}{dt} = \frac{\partial}{\partial x} \), where the condensate energy,
\[ E = E_K + E_P + E_{NL} + E_{DD}, \]
is an integral of motion: \( \frac{dE}{dt} = 0 \), and
\[ E_K = \int \frac{\hbar^2}{2m} |\nabla \Psi|^2 d^3r, \]
\[ E_P = \int \frac{1}{2} m\omega_x^2 (x_1^2 + x_2^2 + \gamma^2 x_3^2) |\Psi|^2 d^3r, \]
\[ E_{NL} = \frac{g}{2} \int |\Psi|^4 d^3r, \]
\[ E_{DD} = \frac{1}{2} \int |\Psi(r)|^2 \left[V(r - r') - V(r')\right] |\Psi(r')|^2 d^3r \cdot d^3r'. \]

Consider time evolution of the mean square radius of the wave function, \( \langle r^2 \rangle \equiv \int r^2|\Psi|^2 d^3r/N \). Using \( \text{(2)} \), integrating by parts, and taking into account vanishing boundary conditions at infinity one gets for the first time derivative
\[ \partial_t \langle r^2 \rangle = \frac{\hbar}{2mN} \int 2i x_j (\Psi \partial_{x_j} \Psi^* - \Psi^* \partial_{x_j} \Psi) d^3r, \]
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, \( j = 1, \ldots, 3 \).

In a similar way, after a second differentiation over \( t \), one gets
\[ \partial_t^2 \langle r^2 \rangle = \frac{1}{2mN} \left[ 8E_K - 8E_P + 12E_{NL} \right. \\
-2 \left. \int |\Psi(r)|^2 |\Psi(r')|^2 (x_j \partial_{x_j} x_j' \partial_{x_j'} V(r - r') d^3r). \right. \]
\[ \left. \right. \]
\[ \left. \right. \]Note that, in the case \( E_P = 0 \), \( V(r) \equiv 0 \), Eq. \( \text{(1)} \) coincides with the so-called virial theorem for the GPE with local interactions \( \text{(1), (2), (3), (4), (6)} \) thus it is natural to call Eq. \( \text{(1)} \) by a virial theorem for GPE \( \text{(1)} \).

Using Eq. \( \text{(2)} \), one gets \( (x_j \partial_{x_j} x_j') V(r - r') = -3V(r - r') \) and using Eq. \( \text{(3)} \) one can rewrite virial theorem \( \text{(3)} \) as follows:
\[ \partial_t^2 \langle r^2 \rangle = \frac{1}{2mN} \left[ 12E - 4E_K - 10m\omega_0^2 N \langle r^2 \rangle \right. \\
-10m\omega_0^2 N(\gamma - 1) (x_3^2) \left. \right]. \]
\[ \text{(7)} \]

It is essential here that both local nonlinear term and nonlocal term are included into the energy which is a conserved quantity. Catastrophic collapse of BEC occurs while \( \langle r^2 \rangle \to 0 \). From mathematical point of view it means that if, according to virial theorem \( \text{(3)} \), the positive-definite quantity \( \langle r^2 \rangle \) becomes negative in finite time then singularity in solution of Eq. \( \text{(3)} \) appears in a finite time before \( \langle r^2 \rangle \) becomes negative and singularity in solution of GPE occurs together with catastrophic squeezing of the distribution of \(|\Psi|\). Near singularity formation GPE is not applicable and another physical mechanisms are important such as inelastic two- and three-body collisions which can cause a loss of atoms from the condensate \( \text{(3)} \). In addition, long term interactions are described by the dipole-dipole potential \( \text{(3)} \) provided typical distance between atoms in condensate exceeds a few Bohr radii. Note that regularization of potential \( \text{(2)} \) to avoid singularity at \( r = 0 \) allows to prevent singularity formation in GPE \( \text{(13, 20)} \). However GPE \( \text{(1)} \) can still describe significant contraction of atomic cloud.

Thus condition \( \langle r^2 \rangle \to 0 \) provides a sufficient criterion of collapse of BEC. E.g., one immediately obtains from Eq. \( \text{(7)} \) that \( \partial_t^2 \langle r^2 \rangle < \frac{\hbar^2}{mE} \) and collapse is inevitable for \( E < 0 \). One can obtain however much more strict sufficient condition for collapse using generalized uncertainty relations between \( E_K, N, \langle r^2 \rangle, \partial_t \langle r^2 \rangle \) which follows from Cauchy-Schwarz inequality and Eq. \( \text{(3)} \) with use of integration by parts \( (\Psi = R e^{i\phi}, R = |\Psi|)\):
\[ E_K = \frac{\hbar^2}{2m} \int \left[ (\nabla R)^2 + (\nabla \phi)^2 R^2 \right] d^3r, \]
\[ \frac{2mN}{\hbar} |\partial_t \langle r^2 \rangle| = 4 \int x_j \partial_{x_j} x_j R \frac{d^3r}{\sqrt{2}} \leq 4 \left( N \langle r^2 \rangle \right)^{1/2} \left( \nabla \phi \right)^2 R^2 d^3r \]
\[ N = -\frac{2}{3} \int x_j R \partial_{x_j} x_j R d^3r \leq \frac{2}{3} \left( N \langle r^2 \rangle \right)^{1/2} \left( \nabla R \right)^2 d^3r. \]
Using Eqs. \( \text{(7)}, \text{(8)} \) one can obtain a basic differential inequality:
\[ \partial_t^2 \langle r^2 \rangle \leq \frac{1}{2mN} \left[ 12E - \frac{\hbar^2}{2m} \left( \frac{9N}{r^2} + \frac{m^2 N (\partial_t \langle r^2 \rangle)^2}{\hbar^2} \right) \right. \\
-10m\omega_0^2 N F(\gamma) \langle r^2 \rangle], \]
\[ \text{(9)} \]
where \( F(\gamma) = 1 \) for \( \gamma \geq 1 \) and \( F(\gamma) = \gamma^2 \) for \( \gamma < 1 \). Change of variable, \( \langle r^2 \rangle = B^{1/5}/N \) gives the differential inequality:
\[ \partial_t^2 B \leq \frac{5}{2m} \left[ 3EB^{1/5} - \frac{\hbar^2}{8m} \frac{9N^2}{B^{3/5}} - \frac{5}{2} m\omega_0^2 F(\gamma) B \right], \]
\[ \text{(10)} \]
which can be rewritten as
\[ B_{tt} = -\frac{\partial U(B)}{\partial B} - f^2(t), \]
\[ \text{(11)} \]
where

\[ U = -\frac{25}{4m} E B^6/5 + \frac{\hbar^2 225 N^2}{32m^2} B^2/5 + \frac{25}{8} \omega_0^2 F(\gamma) B^2, \tag{12} \]

and \( f^2(t) \) is some unknown nonnegative function of time.

Equation (11) has a simple mechanical analogy with the motion of a “particle” with coordinate \( B \) under the influence of the potential force \( -\partial U(B) / \partial B \), in addition to the force \( -f^2(t) \). Due to the influence of the nonpotential force \( -f^2(t) \) the total energy \( E \) of the “particle” is time dependent: \( E(t) = E(0) + U(B) \). Collapse certainly occurs if the “particle” reaches the origin \( B = 0 \). It is clear that if the particle were to reach the origin without the influence of the force \( -f^2(t) \) then it would reach the origin even faster under the additional influence of this nonpotential force. Therefore one can consider below the particle dynamics without the influence of the nonconservative force \( -f^2(t) \) to prove sufficient collapse conditions.

It follows from (12) that potential \( U(B) \) is a monotonic function for \( E \leq \hbar \omega_0 N F(\gamma) / 5 \) \( 1/2 / 2 = E_{\text{critical}} \) (see curve 1 in Fig. 1) while for \( E > E_{\text{critical}} \) potential \( U(B) \) has a barrier at \( B_m^1 \) \( 1/5 = 3 \left( E - E_{\text{critical}} \right)^{1/2} / \left[ 5m \omega_0^2 F(\gamma) \right] \) with particle energy \( E_m = U(B_m) \) at the top (see curve 2 in Fig. 1). One can separate sufficient collapse condition into three different cases:

(a) for \( E \leq E_{\text{critical}} \) the particle reaches the origin in a finite time irrespective of the initial value of \( B|_{t=0} \);

(b) for \( E > E_{\text{critical}} \) and \( E(0) > E_m \), the particle is able to overcome the barrier thus it always falls to the origin in a finite time irrespective of the initial value of \( B|_{t=0} \);

(c) for \( E > E_{\text{critical}} \) and \( E(0) < E_m \), the particle is not able to overcome the barrier thus it falls to the origin in a finite time only if \( B|_{t=0} < B_m \).

Note that it is proven here analytically only sufficient collapse conditions. It means that even if none of conditions \( a,b,c \) are satisfied one can not exclude collapse formation for some particular values of the initial conditions of Eq. (1). Generally it is determined by nonpotential force \( -f^2(t) \). However inequality (4) reduces to equality for a Gaussian initial condition and \( \gamma = 1 \):

\[ \Psi_0 = N^{1/2} \pi^{-3/4} (L_\rho L_3)^{-1/2} e^{-(x_1^2 + x_2^2)/2L_\rho^2} e^{-x_3^2/2L_3^2}. \tag{13} \]

in particular case with \( L_3 = L_\rho \).

One can compare sufficient collapse condition with results of Ref. [8] where collapse was predicted from variational analysis using Gaussian ansatz (13) to approximate ground state of GPE for \( g = 0 \) (1). It was concluded that collapse should occur provided energy functional \( E \) has no local minima. A critical point was determined from the condition that local minimum of energy functional \( E \) becomes a saddle point:

\[ \frac{\partial^2 E}{\partial L_3^2} \frac{\partial^2 E}{\partial L_\rho^2} = 0. \]

This allows to find critical number of particle, \( N_{\text{var}} \) and critical value of energy functional, \( E_{\text{var}} \), as a function of system parameters \( L_\rho, L_3, \gamma, d, \ldots \).

Fig. 2 shows dependence of \( E_{\text{var}} \) (curve 1) and \( E_{\text{critical}} \) (curve 2) on trap aspect ratio \( \gamma \) for \( N = N_{\text{var}} \). Both \( E_{\text{var}} \) and \( E_{\text{critical}} \) are given in units of \( \hbar^2 / (m \omega_0)^{5/4} \).
potential (2) allows to find a sufficient condition of global existence (for arbitrary large time) of solution of GPE (1). The dipole-dipole interaction energy $E_{DD}$ can be rewritten in k-space as $E_{DD} = (1/2) \int |R_k|^2 V_k d^3k/(2\pi)^3$, where $R_k$ is a Fourier transform of $|\Psi|^2$ and the Fourier transform of the dipole-dipole interaction in the limit of small atomic overlap distance is given by $V_k = -\frac{\pi}{2d^2}(1 - 3\cos^2 \alpha)$. Here $\alpha$ is the angle between $k$ and $d$. Using inequality $V_k \geq -\frac{\pi d^2}{2}$ one gets $E_{DD} \leq -\frac{\pi d^2}{2} Y$, where $Y = \int |\Psi|^4 d^3r$. Condition $4\pi d^2 < 3g$ results in $E > 0$ for any particle number and collapse is impossible. Below it is assumed that $4\pi d^2 > 3g$. $Y$ can be bounded as follows: $Y \leq \frac{4}{3l^2 N_0} N_1^2/X^3/2$, where $X = \int |\nabla^3 |^2 d^3r$, and $N_0 = 18.94$ is determined from a ground state solution, $\phi_0 = \lambda R(x)e^{i\lambda x}$, of nonlinear Schrödinger equation: $-\lambda^2 R + \nabla^2 R + R = 0$, $N_0 = \int R^2 d^3r$ (see Ref. 23). Using these inequalities and Eqs. 3, 4, 5 one gets lower bound of energy functional:

$$E \geq \frac{\hbar^2}{2m} X + \frac{9m_0}{8X} F(\gamma) N^2 - 2(4\pi d^2 - 3g) N_0^{3/2} X^3/2 \equiv E_0(X)$$

For $N > N_c$, $E_0 = \frac{2^{3/2} 3h^5/2 N_0}{5^{5/4} (4\pi d^2 - 3g) F(\gamma)^{1/4} m^{3/2} \omega^{3/2}}$, the function $E_0(X)$ is a monotonic one (curve 1 in Fig. 3). For $N < N_c$ the function $E_0(X)$ has a local minimum, $E_{min}$ (curve 2 in Fig. 3). Consider initial condition with

$$N < N_c, \quad E_{min} < E < E_{max}, \quad X_1 < X < X_2,$$

where $E_{max}$ is a local maximum of $E_0(X)$, and $X_1, X_2$ are two of total three roots ($X_1 < X_2 < X_3$) of Eq. $E = E_0(X)$. Any solution of GPE, corresponding to conditions (15), will stay in the range $X_1 < X < X_2$ at any time because regions below curves 1, 2 in Fig. 3 are forbidden for solution of GPE. One concludes that collapse is impossible in that case because collapse and singularity formation in GPE requires singularity in kinetic energy $X \to \infty$. That could be understood e.g. from uncertainty relations (3). Eq. (16) gives a sufficient condition of absence of collapse and in that case one can expect that energy functional $E$ has a local minimum and supports stable steady-state solutions. In original quantum mechanical problem that steady state is metastable one because of finite probability of tunneling of condensate from local minimum which is outside the applicability of GPE and is not considered in this Letter.

In conclusion, sufficient analytical criteria are developed both for catastrophic collapse of BEC of gas with nonlocal long-range dipole-dipole interactions and for long-time collapse existence in the framework of GPE (1).

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