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Collapse of Bose-Einstein condensates with dipole-dipole interactions

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The dynamics of Bose-Einstein condensates 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 condensates 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 have been 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 one to achieve a metastable Bose-Einstein condensate (BEC) [2] for $a<0$ if the number of particles is small enough to ensure the existence of local minima of the energy functional [3].

Recent progress in creating of ultracold molecular clouds [4,5] opens a new prospective for achieving BEC in a dilute gas of polar molecules and stimulates a growing interest in the study of BEC with dipole-dipole interactions [6–12]. Dipole-dipole forces are long range and essentially anisotropic. The 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. Thus stability and collapse of BEC strongly depend on clouds anisotropy which opens a whole bunch of new phenomena to be observed and makes the task of achieving and controlling the 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 [6,9]. Another possible physical realization is atoms with laser induced electric dipole moments [8]. Dipole-dipole interactions can be also essential in BEC of atomic gas with large magnetic dipole moments [7,11]. Magnetic interactions are usually dominated by van der Waals forces but effects of magnetic interactions can be essentially amplified by reducing scattering length a via a Feshbach resonance [13,10]. Analysis of this paper can be applied for both cases of electric and magnetic dipole-dipole interactions.

In this paper 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 allow one to predict condensate collapse or, contrarily, 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 the variational approach [8], where collapse was predicted based on the absence of a local minimum of the ground state of the energy functional provided number of condensate particle exceeds a certain critical value. It is shown here that variational calculation gives a threshold number of particles and condensate energy which are located between parameter regions where analytical criteria predict collapse and long-time condensate existence, respectively. It is proven in this paper that collapse certainly occurs provided energy of the condensate is below a threshold value which is determined by the number of particles and trap parameters. Collapse of the condensate is accompanied by a dramatic contraction of the atomic cloud. Collapse is impossible provided the 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 [6]

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

where $\mathbf{r}=(x_1,x_2,x_3)$, Ψ is the condensate wave function, coupling constant g corresponds to short-range forces and is given by $g=4\pi\hbar^2a/m$, a is the *s*-wave scattering length, m is the atomic mass, ω_0 is a trap frequency in the x_1x_2 plane, and γ is the anisotropy factor of the trap. $\Psi(\mathbf{r},t)$ is normalized to the total number of atoms in condensate: $N=\int|\Psi|^2d^3\mathbf{r}$. It is assumed that the system is away from shape resonances of $V(\mathbf{r})$ [6] and that the long-range potential is due to the dipole-dipole interaction, and is given by

$$V(\mathbf{r}-\mathbf{r}')=\frac{[\mathbf{d}_1(\mathbf{r})\cdot\mathbf{d}_2(\mathbf{r}')]-3[\mathbf{d}_1(\mathbf{r})\cdot\mathbf{u}][\mathbf{d}_2(\mathbf{r}')\cdot\mathbf{u}]}{|\mathbf{r}-\mathbf{r}'|^3}, \tag{2}$$

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where $\mathbf{u}=(\mathbf{r}-\mathbf{r}')/|\mathbf{r}-\mathbf{r}'|$. All the dipoles are assumed to point in the direction of trap axes ($\hat{x}_3$ direction), i.e., $\mathbf{d}_1=\mathbf{d}_2=d\hat{x}_3$. Potential (2) with no dependence of d on $\mathbf{r}$ is a good approximation provided a typical interparticle distance exceeds a few Bohr radii.

GPE (1) can be also obtained from variation of energy functional, E: $i\hbar(\partial\Psi/\partial t)=\delta E/\delta\Psi^*$, where the condensate energy

$$E=E_K+E_P+E_{NL}+E_{DD} \tag{3}$$

is an integral of motion $dE/dt=0$, and

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

Consider time evolution of the mean-square radius of the wave function, $\langle r^2\rangle\equiv\int r^2|\Psi|^2d^3\mathbf{r}/N$. Using Eq. (1), integrating by parts, and taking into account vanishing boundary conditions at infinity one gets for the first time derivative,

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

where $\partial_t\equiv\partial/\partial t$, $\partial_{x_j}\equiv\partial/\partial x_j$, and repeated index j means summation over all space coordinates, $j=1,\dots,3$.

In a similar way, after a second differentiation over t, one gets

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

Note that, in the case $E_P=0, V(\mathbf{r})\equiv 0$, Eq. (6) coincides with the so-called virial theorem for the GPE with local interactions [14–18] and thus it is natural to call Eq. (6) by a virial theorem for GPE (1).

Using Eq. (2) one gets $(x_j\partial_{x_j}+x_j'\partial_{x_j'})V(\mathbf{r}-\mathbf{r}')=-3V(\mathbf{r}-\mathbf{r}')$ and using Eq. (3) one can rewrite virial theorem (6) as follows:

$$\begin{aligned}\partial_t^2\langle r^2\rangle=\frac{1}{2mN}[&12E-4E_K-10m\omega_0^2N\langle r^2\rangle\\ &-10m\omega_0^2N(\gamma^2-1)\langle x_3^2\rangle].\end{aligned} \tag{7}$$

It is essential here that both local nonlinear term and nonlocal term are included into the energy E which is a conserved quantity. Catastrophic collapse of BEC occurs while $\langle r^2\rangle\to 0$. From a mathematical point of view it means that if, according to virial theorem (7), the positive-definite quantity $\langle r^2\rangle$ becomes negative in a finite time then singularity in the solution of Eq. (1) appears in a finite time before $\langle r^2\rangle$ becomes negative and singularity in the solution of the GPE occurs together with catastrophic squeezing of the distribution of $|\Psi|$. Near singularity formation GPE is not applicable and other physical mechanisms are important such as inelastic two- and three-body collisions which can cause a loss of atoms from the condensate [3]. In addition, long term interactions are described by the dipole-dipole potential (2) provided the typical distance between atoms in condensate exceeds a few Bohr radii. Note that the regularization of potential (2) to avoid singularity at $r=0$ allows to prevent singularity formation in the GPE [19,20]. However, GPE (1) can still describe the significant contraction of the atomic cloud.

Thus condition $\langle r^2\rangle\to 0$ provides a sufficient criterion of collapse of BEC. For example, one immediately obtains from Eq. (7) that $\partial_t^2\langle r^2\rangle<6E/mN$ and collapse is inevitable for $E<0$. One can obtain however a much more strict sufficient condition for collapse using generalized uncertainty relations between $E_K, N, \langle r^2\rangle, \partial_t\langle r^2\rangle$ [16] which follows from the Cauchy-Schwarz inequality and Eq. (5) with use of integration by parts ($\Psi\equiv Re^{i\phi}$, $R=|\Psi|$),

$$\begin{gathered}E_K=\frac{\hbar^2}{2m}\int[(\nabla R)^2+(\nabla\phi)^2R^2]d^3\mathbf{r},\\ \frac{2mN}{\hbar}|\partial_t\langle r^2\rangle|=4\left|\int x_j\partial_{x_j}\phi R^2d^3\mathbf{r}\right|\\ \leqslant 4\left(N\langle r^2\rangle\int(\nabla\phi)^2R^2d^3\mathbf{r}\right)^{1/2},\\ N=-\frac{2}{3}\int x_jR\partial_{x_j}Rd^3\mathbf{r}\leqslant\frac{2}{3}\left(N\langle r^2\rangle\int(\nabla R)^2d^3\mathbf{r}\right)^{1/2}.\end{gathered} \tag{8}$$

Using Eqs. (7) and (8) one can obtain a basic differential inequality,

$$\begin{aligned}\partial_t^2\langle r^2\rangle\leqslant\frac{1}{2mN}\bigg[&12E-\frac{\hbar^2}{2m}\left(\frac{9N}{\langle r^2\rangle}+\frac{m^2N(\partial_t\langle r^2\rangle)^2}{\hbar^2\langle r^2\rangle}\right)\\ &-10m\omega_0^2NF(\gamma)\langle r^2\rangle\bigg],\end{aligned} \tag{9}$$

where $F(\gamma)=1$ for $\gamma\geqslant 1$ and $F(\gamma)=\gamma^2$ for $\gamma<1$. Function $F(\gamma)$ originates from estimate of upper bound of term $-\langle r^2\rangle-(\gamma^2-1)\langle x_3^2\rangle\leqslant -F(\gamma)\langle r^2\rangle$ in Eq. (7). Change of variable, $\langle r^2\rangle=B^{4/5}/N$ gives the differential inequality,

$$\partial_t^2B\leqslant\frac{5}{2m}\left[3EB^{1/5}-\frac{\hbar^2}{8m}\frac{9N^2}{B^{3/5}}-\frac{5}{2}m\omega_0^2F(\gamma)B\right], \tag{10}$$

which can be rewritten as

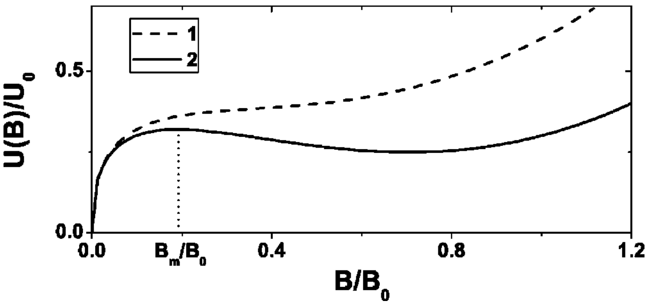

FIG. 1. Typical behavior of potential $U(B)$ from Eq. (12) for $E \leqslant E_{critical}$ (curve 1) and $E > E_{critical}$ (curve 2). $U_0 = (N^5\hbar^5/m^5\omega_0)^{1/2}$, $B_0 = (N\hbar/m\omega_0)^{5/4}$.

$$B_{tt} = -\frac{\partial U(B)}{\partial B} - f^2(t), \tag{11}$$

where

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

and $f^2(t)$ is some unknown non-negative function of time. Equation (11) has a simple mechanical analogy [16] 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 $\mathcal{E}$ of the particle is time dependent: $\mathcal{E}(t) = B_t^2/2 + U(B)$. 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 nonpositive 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 Eq. (12) that potential $U(B)$ is a monotonic function for $E \leqslant \hbar\omega_0 N[F(\gamma)5]^{1/2}/2 \equiv E_{critical}$ (see curve 1 in Fig. 1) while for $E > E_{critical}$ potential $U(B)$ has a barrier at $B_m^{4/5} = 3(E - [E^2 - E_{critical}^2]^{1/2})/[5m\omega_0^2 F(\gamma)]$ with particle energy $\mathcal{E}_m = U(B_m)$ at the top (see curve 2 in Fig. 1). One can separate sufficient collapse condition into three different cases.

(a) For $E \leqslant E_{critical}$ the particle reaches the origin in a finite time irrespective of the initial value of $B|_{t=0}$.

(b) For $E > E_{critical}$ and $\mathcal{E}(0) > \mathcal{E}_m$, 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 $E > E_{critical}$ and $\mathcal{E}(0) < \mathcal{E}_m$, 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 the conditions (a)–(c) are satisfied one cannot 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 (9) reduces to equality for a Gaussian initial condition and $\gamma = 1$,

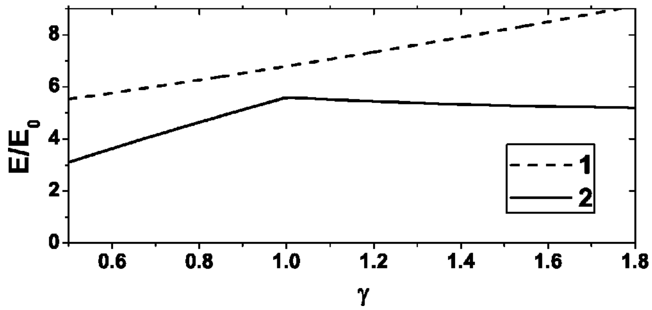

FIG. 2. Dependence of $E_{c,\,var}$ (curve 1) and $E_{critical}$ (curve 2) on trap aspect ratio γ for $N = N_{c,\,var}$. Both $E_{c,\,var}$ and $E_{critical}$ are given in units of $E_0 = \hbar^{7/2}\omega_0^{1/2}/d^2 m^{3/2}$.

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

in particular the case with $L_3 = L_\rho$.

One can compare the sufficient collapse condition with results of Ref. [8] where collapse was predicted from a variational analysis using the Gaussian ansatz (13) to approximate ground state of the 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: $(\partial^2 E/\partial L_3^2)(\partial^2 E/\partial L_\rho^2) = (\partial^2 E/\partial L_3 \partial L_\rho)^2$, $\partial E/\partial L_3 = \partial E/\partial L_\rho = 0$. This allows one to find the critical number of particles, $N_{c,var}$, and critical value of energy functional, $E_{c,var}$, as a function of system parameters L_ρ, L_3, γ, d. Figure 2 shows the dependence of $E_{c,\,var}$ (curve 1) and $E_{critical}$ (curve 2) on trap aspect ratio γ for $N = N_{c,\,var}$ and $g = 0$. Note that the expression for $E_{c,\,var}$, used in this paper to draw curve 2 in Fig. 2, differs from Eq. (3) of Ref. [8]. The authors of Ref. [8] already mentioned in the erratum [21] that Eq. (3) of Ref. [8] is incorrect. However, a corrected formula was not given in the erratum [21]. The explicit expression for $E_{c,\,var}$ is not given in this paper also because it is very bulky and will be given elsewhere. The Gaussian ansatz (13) is not an exact solution of the GPE (1); thus one can expect that actual critical value of energy E of the ground-state solution is lower. $E_{critical}$ is determined here from the sufficient collapse condition meaning that the critical value of energy E of the ground-state solution is always above curve 2. One can conclude that the actual critical value of energy is located between curves 1 and 2. The accuracy of the variation approximation can generally be obtained only from comparison with direct simulation of the GPE (1).

The Fourier transform of dipole-dipole interaction potential (2) allows one to find a sufficient condition of global existence (for arbitrary large time) of the solution of the GPE (1). The dipole-dipole interaction energy E_{DD} can be rewritten in **k** space as $E_{DD} = (1/2)\int |R_{\mathbf{k}}|^2 V_{\mathbf{k}} d^3\mathbf{k}/(2\pi)^3$, where $R_{\mathbf{k}}$ 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 Ref. [7]: $V_{\mathbf{k}} = -(4\pi/3)d^2(1 - 3\cos^2\alpha)$. Here α is the angle between **k** and **d**. Using the inequality $V_{\mathbf{k}} \geqslant -(4\pi/3)d^2$ one gets $E_{DD} \geqslant -(2\pi/3)d^2 Y$, where $Y \equiv \int |\Psi|^4 d^3\mathbf{r}$. Condition $4\pi d^2 \leqslant 3g$ 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: $Y\leqslant(4/3^{3/2}N_0)N^{1/2}X^{3/2}$, where $X\equiv\int|\nabla\Psi|^2d^3\mathbf{r}$, and $N_0=18.94$ is determined from a ground state solution, $\phi_0=\lambda R(\lambda\mathbf{r})e^{i\lambda^2t}$, of nonlinear Schrödinger equation, $-\lambda^2R+\nabla^2R+R^3=0$, $N_0\equiv\int R^2d^3\mathbf{r}$ (see Ref. [23]). Using these inequalities and Eqs. (3), (4), and (8) one gets the lower bound of the energy functional,

$$E\geqslant\frac{\hbar^2}{2m}X+\frac{9m\omega^2}{8X}F(\gamma)N^2-\frac{2(4\pi d^2-3g)}{3^{5/2}N_0}N^{1/2}X^{3/2}\equiv E_l(X). \quad (14)$$

For $N>N_c$, $N_c\equiv2^{3/2}3\hbar^{5/2}N_0/[5^{5/4}(4\pi d^2-3g)F(\gamma)^{1/4}m^{3/2}\omega^{1/2}]$, the function $E_l(X)$ is a monotonic one (curve 1 in Fig. 3). For $N<N_c$ the function $E_l(X)$ has a local minimum, E_{min} (curve 2 in Fig. 3). Consider the initial condition with

$$N<N_c,\quad E_{min}<E<E_{max},\quad X_1<X|_{t=0}<X_2, \quad (15)$$

where E_{max} is a local maximum of $E_l(X)$, and X_1,X_2 are two of a total of three roots ($X_1<X_2<X_3$) of the equation $E=E_l(X)$. Any solution of the 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 require singularity in kinetic energy [22], $X\to\infty$. That could be understood, e.g., from uncertainty relations (8).

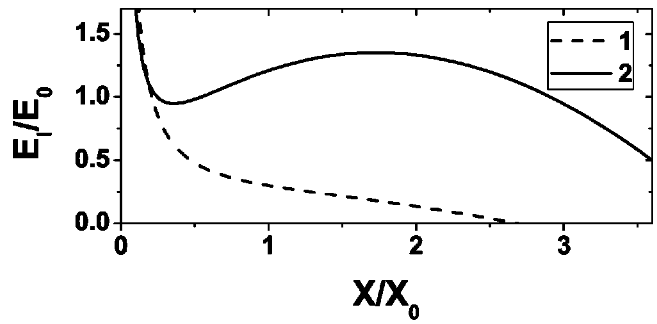

FIG. 3. Energy lower bound E_l (in units of E_0) for $N>N_c$ (curve 1) and $N<N_c$ (curve 2) versus X/X_0. $X_0=N^{3/5}[mN_0\omega_0^2/(4\pi d^2-3g)]^{2/5}$.

Equation (15) 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 paper.

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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