Collapse of the metastable state in an attractive Bose-Einstein condensate

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The characteristic features of the collapse of the ground state in trapped one-component attractive Bose-Einstein condensates are studied by applying the catastrophe theory. From numerically obtained stable and unstable solutions of the Gross-Pitaevskii equation, we derive the catastrophe function defining the stability of the stationary points on the Gross-Pitaevskii energy functional. The bifurcation diagram and the universal scaling laws stemming from the catastrophe function show quantitative agreement with the numerical results.

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The experimental observation of Bose-Einstein condensation (BEC) in ultracold atomic gases [1,2] has stimulated immense interests in the study of the macroscopic quantum phenomena. One of the central issues in the field of BEC is to understand how the interparticle interaction influences the ground state of BEC. In this respect, recent realization of BEC in Li atomic gases [3] has invoked special interests since it is expected to show the collapse behavior when the number of particles \( N \) in the condensate exceeds a critical value \( N_{cr} \) [4]. The collapse of trapped BEC stands in contrast to the well-known homogeneous system in which the condensate is always unstable for the attractive interaction [5].

First qualitative insight into the collapse behaviors was obtained by the variational approach based on the Gaussian approximation [6]. It shows that the condensate is in the metastable state below \( N_{cr} \) corresponding to a minimum of the Gross-Pitaevskii energy functional (GPEF). Above \( N_{cr} \), the minimum disappears and corresponding Gross-Pitaevskii equation (GPE) has no solution.

More advanced description for the collapse of BEC was presented by Huepe et al. [7]. They computed the branches of the stable and unstable solutions of the GPE, and found that these meet at a critical particle number through the Hamiltonian saddle node (HSN) bifurcation. Within sufficiently narrow range around the critical point, the HSN bifurcation describes the essential features of the collapse behavior. For the system following the HSN bifurcation, the bifurcation function must be symmetric with respect to the control parameter, \( x = 1 - N/N_{cr} \). Also, the critical amplitude, which was defined as the one related to the radius of the condensate [7], does not show symmetric behavior predicted by the HSN bifurcation. To maintain the symmetry, the catastrophe function governing the bifurcation has to retain the odd symmetry with respect to the critical amplitude [8]. Our study shows that the catastrophe function indeed has additional even terms, which is essential to describe the asymmetric nature of the bifurcation.

The condensate in a radially symmetric trap is described by the GPEF,

\[
E[\psi; g, N] = \int d\mathbf{r} \psi^* \left[ -\nabla^2/2 + r^2/2 + gN/2|\psi|^2 \right] \psi,
\]

where \( g \) is a pseudopotential between the trapped atoms defined by \( 4\pi a_s/l_0 \), \( a_s \), and \( l_0 = \sqrt{\hbar/m\omega} \) being the s-wave scattering length and the harmonic oscillator length, respectively. We scaled the length and the energy with respect to \( l_0 \) and \( \hbar \omega \), respectively. The stationary solutions of Eq. (1) has been calculated by solving the GPE, \( [-\nabla^2/2 + r^2/2 + gN|\psi|^2] \psi = \mu \psi \), where the Lagrange multiplier \( \mu \) is introduced to preserve the number of particle \( N \). In previous works [9,10,11], the stability of the ground state of the condensate has been studied by computing the excitation frequencies of the Hartree-Fock equation. Here we examine the stability of the condensate by calculating the eigenvalues of the Hessian matrix of the GPEF. The bifurcation pattern stemming from the critical point can be obtained by investigating how the stability of the stationary solutions of \( E[\psi; g, N] \) changes as a function of the control parameters \( g \) and \( N \) [11].

By setting \( \psi(r) = \phi(r)/r \) and dividing the space into grids by approximating \( \phi(r) \) by \( \phi_l \) for \( l \delta < r < (l+1) \delta \), where \( \delta \) is the mesh length in a radial direction, the GPEF becomes

\[
E[\phi_l] = A_1 \sum_l \phi_l (\phi_{l+1} - 2 \phi_l + \phi_{l-1}) + A_2 \sum_l l^2 \phi_l^2 + N A_3 \sum_l \phi_l^4 / l^2,
\]

(2)

where \( A_1 = -2\pi/\delta \), \( A_2 = 2\pi^3/\delta^2 \), and \( A_3 = 2\pi g/\delta \). The discrete form of the GPE is also given by

\[
A_1 (\phi_{l+1} - 2 \phi_l + \phi_{l-1}) + A_2 l^2 \phi_l + 2 N A_3 \phi_l^4 / l^2 = \mu \phi_l.
\]

(3)

Comprehensive explanations on numerical techniques constructing the solution of the GPE can be found in Ref. [12]. Therefore, only a brief explanation is presented. We first determine a trial solution \( \phi_l \) for an arbitrary \( N \) and \( \mu \) from the recursion relation Eq. (3). Next, we scale \( \phi_l \) and \( N \) with \( \epsilon = \Sigma_l \phi_l^2 \) as \( \epsilon' = \epsilon N \) and \( \phi_l' = \phi_l / \sqrt{\epsilon} \), respectively. Then we obtain a true solution \( \phi_l' \) for \( \epsilon' \) and \( \mu \). In Fig. 1(a) we plot the energies for the stable \( E^+ \) and unstable solutions \( E^- \) as functions of \( N \), respectively.

The stabilities of the stationary solutions are determined from the eigenvalues of the Hessian of the GPEF. Consider-
where $\Phi$ is the Morse function depending on the number of zero eigenvalues and the number of the control parameters $N_{cr}$. In addition, $\lambda_2^{proj}$ and $\lambda_{HB}$ become imaginary, which means an exponential growth of the fluctuations with a time evolution.

The canonical forms of the catastrophe function depend on the number of zero eigenvalues and the number of the control parameters [8]. Since our system has single zero eigenvalue $\lambda_2^{proj}$ and one control parameter $N$, the local geometry of the GPEF follows the fold catastrophe whose normal form can be written as a cubic polynomial with respect to a critical amplitude. However, it is almost intractable to derive the canonical form of the catastrophe function analytically from the original energy functional $E$ in such a high-dimensional system. Instead, we first propose the functional form of the catastrophe function from the GPEF, and determine the scaling parameters by numerical fitting. The Taylor expansion of the GPEF around $\Phi_0$ and $N_{cr}$, where $\Phi_0$ is the solution of the GPE at the bifurcation point $N_{cr}$, gives

$$E[\Phi,x]=E_0[\Phi_0,0]-xN_{cr}A_3\sum_l(\phi_l^0)^4/l^2$$

$$+N_{cr}\left[-x4A_2\sum_l(\phi_l^0)^3/l^2\delta\phi_l +\delta\Phi^{\prime\prime}\mathbf{H}^{proj}\delta\Phi^{\prime}\right]$$

$$-x6A_3\sum_l(\phi_l^0)^2/l^2\delta\phi_l^2+(1-x)4A_3\sum_l(\phi_l^0)^2/l^2\delta\phi_l^4$$

$$+(1-x)A_2\sum_l\delta\phi_l^4/l^2$$

where $\Phi=\mathbf{P}\delta\Phi^{\prime}$, and $x$ is the control parameter defined as $x=1-N/N_{cr}$. Notice that those fluctuations that satisfy the constraint are allowed only, by projecting $\delta\Phi^{\prime}$ to the constraint subspace. Next, using a linear transformation $\mathbf{P}\delta\Phi^{\prime}\mathbf{P}^T$, where $\mathbf{P}_i=\delta\Phi^{\prime}\mathbf{e}_{\Phi_i}$, Eq. (4) can be rewritten as a function of $Q_i$ ($l=2, \ldots, L$).

$$E[\Phi,x]=E_0-\alpha x+N_{cr}\sum Q_i^2\left[\sum_{i=3}K_iQ_i^2+x\sum_{i=2}K_{ijkl}Q_iQ_jQ_k\right]$$

$$+(1-x)\sum_{i=1}K_iQ_i^2\left[\sum_{ijkl}K_{ijkl}Q_iQ_jQ_kQ_l\right]$$

where $\alpha=N_{cr}A_3\Sigma_{ij}(\phi_l^0)^4/l^2=-0.802$. The projection of $\delta\Phi^{\prime}$ onto the constraint subspace eliminates all terms containing $Q_1$. Also the term $Q_2^4$ does not appear in the first term in the square bracket in Eq. (5) because of $\lambda_2^{proj}=0$. Furthermore, Thom’s splitting lemma [13] enables us to split the terms in Eq. (5) into two parts,

$$E[\Phi,x]=E_0-\alpha x+F_{NM}(Q_2)+F_M[Q_3, \ldots, Q_L]$$

$$=E_0-\alpha x+\beta xQ_2+\gamma xQ_2^2+\delta(1-x)Q_2^3$$

$$+\eta(1-x)Q_2^4+F_M[Q_2, \ldots, Q_L]$$

where $F_{NM}$ is the non-Morse function written in a polynomial form of $Q_2$ with undetermined coefficients, and $F_M$ is the Morse function depending on $Q_l$ ($l=3, \ldots$). The basic idea of our analysis is to reduce $E_0-\alpha x+F_{NM}$ to the catastrophe function with appropriate scaling parameters. Here $Q_2$ is a critical amplitude measuring how far is the system from the bifurcation point. We propose the form of the catastrophe function $F$ as

$$F[Q_2]=E_0-\alpha x+\beta x\kappa^3Q_2+\gamma x\kappa^2Q_2^2$$

$$+\delta(1-x)\kappa^3Q_2^3+\eta(1-x)\kappa^4Q_2^4$$

The energy (a) and the eigenvalue (b) as a function of the bifurcation parameter $x=1-N/N_{cr}$.
where \( \beta, \gamma, \delta, \eta, \) and \( \kappa \) are to be determined from the numerical solutions. The parameter \( \kappa \) is introduced for the correct scaling of energy. Here we would like to emphasize that the catastrophe function \( F(Q_2) \) does not have terms of degree higher than 4 with respect to \( Q_2 \), since the GPEF has up to quartic nonlinear terms [see Eq. (4)].

From the stationary condition \( \partial F/\partial Q_2 = 0 \), we obtain the following three solutions that correspond to the critical solutions of Eq. (7):

\[
Q_2^0 = \kappa \frac{p}{3} \left[ 1 + 2 \sqrt{1 + B_1 t} \cos \left( \frac{1}{3} \tan^{-1} \frac{G(t)}{1 + B_2 t} \right) \right] \\
= \kappa \frac{p}{3} [1 + Z_0], \\
Q_2^\pm = \kappa \tilde{Q}_2^\pm \\
= \kappa \frac{p}{3} [1 + Z_0/2(1 \pm \sqrt{1 - (2p/3Z_0)^2(1 + B_2 t)})],
\]

where \( B_1 = -3q/p^2, B_2 = -(27/2p^3)(pq/3 + r) \), and \( G(t) = (3B_1 - 2B_2)t + (3B_1^2 - B_2^2)t^2 + B_2^3 t^3, t = x/(1 - x) \). Notice that \( Q_2^0 \) has no physical meaning since it approaches \( \kappa p \) as \( x \to 0 \), which is nonvanishing. Since the critical amplitude \( Q_2 \) corresponds to the order parameter measuring the distance from the bifurcation point, it should be zero at the bifurcation point. In Eq. (8), \( Q_2^\pm \) and \( Q_2^\pm \) correspond to the stable and unstable branches of Eq. (3), respectively. Let us define \( \Delta_{Q_2}(x) = (\Phi_\pm - \Phi_0) \cdot e_{k_{proj}}, \) where \( \Phi_\pm \) is the solution of Eq. (3) for a certain value of control parameter \( x \). Then the parameters \( p, B_1, \) and \( B_2 \) are obtained by fitting \( \tilde{Q}_2^\pm \) to the numerically computed \( \Delta_{Q_2}(x) \) for the stable (unstable) branch. Still the value of \( \kappa \) remains to be determined from the scaling of the energy. In Fig. 2(a), we plot \( \tilde{Q}_2^\pm \) and \( \Delta_{Q_2}(x) \) for the stable and unstable branches with respect to \( x \), respectively. The \( \tilde{Q}_2^\pm \) shows good agreements with the numerically obtained \( \Delta_{Q_2}(x) \) including asymmetric behaviors for a wide range of \( x (\sim <0.03) \). The eigenvalues \( \lambda^\pm \) are obtained by differentiating Eq. (7) twice with respect to \( Q_2 \),

\[
\lambda^\pm = 12N_{cr} \xi(1 - x) [qt/3 - 2p/3\tilde{Q}_2^\pm + (\tilde{Q}_2^\pm)^2],
\]

where \( \xi = \eta \kappa^2 \). Here \( \xi \) is determined by identifying the numerical values of \( \lambda_{proj}^\pm \) for the stable branch with \( \lambda^+ \). We confirmed that the same \( \xi \) is obtained by identifying \( \lambda_{proj}^\pm \) of the unstable branch with \( \lambda^- \). Both \( \lambda^+ \) and \( \lambda^- \) are compared with exact \( \lambda_{proj}^\pm \) obtained from the branches of stable and unstable solutions, respectively, in Fig. 2(b). Finally, the parameter \( \kappa \) is determined by fitting

\[
F[Q_2^+] = E_0 - ax + (1 - x) \xi \kappa^2 [qrt\tilde{Q}_2^+ + 2qt(\tilde{Q}_2^+)^2 \\
- 4p/3(\tilde{Q}_2^+)^3 + (\tilde{Q}_2^+)^4]
\]
to \( E^+ \) of the stable branch. Figure 2(c) shows the profiles of \( F[Q_2^+] \) and \( E^\pm \) as a function of \( x \). The numerical values of the coefficients and scaling parameter are \( \beta = -0.6853, \gamma = 1.345, \delta = 0.6852, \eta = 1.16, \) and \( \kappa = 1.418 \). We plot the catastrophe function \( F[Q_2] \) as a function of \( Q_2 \) in Fig. 3 as control parameter \( x \) varies. The \( F \) shows three optimum points (local maximum, minimum, and global maximum) for \( x > 0 \), two optimum points (saddle and global maximum) for \( x = 0 \), and one global maximum point for \( x < 0 \). For whole range of \( x \), the global maximum corresponding to \( Q_2^0 \) does not correspond to any physically meaningful state. The local structure of \( F \) around \( Q_2 = 0 \) shows the characteristic behavior of collapse of attractive BEC. At the critical point, the local minimum and maximum, which represent the stable \( (Q_2^+) \) and unstable \( (Q_2^-) \) solutions of Eq. (8), are merged into one, and disappear for \( N > N_{cr} \).

Notice that quadratic and quartic terms with respect to \( Q_2 \) in Eq. (7) are proportional to \( \sim x^2 \), whereas linear and cubic terms are proportional to \( \sim x^{3/2} \), since \( Q_2(x) \sim x^{1/2} \) for \( x \ll 1 \). Therefore, within very narrow range of \( x \), our scaling form
can be reduced to the same form predicted by the HSN bifurcation, such as $Q_2^\pm \sim \pm \sqrt{x}$, $\lambda^+ \sim \pm \sqrt{x}$, and $\Delta E = E^- - E^+ \sim x^{3/2}$ by neglecting quadratic and quartic terms with respect to $Q_2^\pm$ in Eq. (7). Next we show that Eq. (7) can be reduced to a canonical form of the fold catastrophe by the nonlinear transformation of $Q_2$. For this purpose, we apply locally diffeomorphic nonlinear transformation, $Q_2(y) = y + \sum_{n=2} D_n y^n$. By substituting $Q_2(y)$ into Eq. (7) and equating the coefficients of $y^n$, we have $F[y] = E_0 - \alpha x + \eta (1 - x) \sum_{n=1} F_n(t) y^n$, where

$$F_1 = \beta \eta, \quad F_2 = \beta D_2 + \gamma,$$

$F_3 = \beta D_3 + 2 \gamma D_2 + \delta,$

$F_4 = \beta D_4 + \gamma (2D_3 + D_2^2) + 3 \delta D_2 + 1,$

$F_5 = \beta D_5 + 2 \gamma D_4 + 3 \delta (D_3 + D_2^2) + 4D_2.$

Here, $\beta = \beta \kappa^2/\eta$, $\gamma = \gamma \kappa^2/\eta$, and $\delta = \delta \kappa/\eta$. The point to be stressed here is that for whole range of $x$, the implicit function theorem guarantees the existence of a smooth invertible transformation $Q_2(y)$, which transforms away all terms of degree greater than 3. At $t=0$, $F[y]$ reduces to $E_0 - \delta \kappa y^3$ by choosing a proper $D_n$. Once $D_2$ is determined as $-1/3 \delta$ from $F_4 = 0$, the transformation coefficients $D_n$ can be chosen to get rid of the term proportional to $y^n$ in $F[y]$ for $n > 3$. For $t \neq 0$, all coefficients $D_n (n > 2)$ are well defined. First, we set $D_2 = - \gamma / \beta$ to remove the quadratic term in $F[y]$. For arbitrary $D_3$ we can make $F_n (n > 4)$ to be zero by choosing a proper $D_n (n > 4)$. The resulting $F(y)$ becomes

$$E_0 - \alpha x + \beta x k^3 y + [(\beta x k^3 D_3 - 2 \gamma^2 \kappa / \beta) x + \delta \kappa (1 - x)] y^3.$$ 

By selecting $D_3 = 2 \gamma^2 / (\beta \kappa)^2$ the canonical form of the fold catastrophe is obtained as $F(y) = E_0 - \alpha x + \beta x k^3 y + \delta (1 - x) \kappa y^3$ with a new critical amplitude $y$.

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