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^{7}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 a proper control parameter. However, in a present system, the eigenvalues of the Hessian matrix of the GPEF shows strong asymmetric behavior 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,

$$E[\psi;g,N]=\int d\mathbf{r}\,\psi^*[-\nabla^2/2+r^2/2+gN/2|\psi|^2]\psi, \quad (1)$$

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 μ 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-Bogoliubov 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 ϕ_l for $l\delta<r<(l+1)\delta$, where δ is the mesh length in a radial direction, the GPEF becomes

$$E[\phi_l]=A_1\sum_l \phi_l(\phi_{l+1}-2\phi_l+\phi_{l+1})+A_2\sum_l l^2\phi_l^2 + NA_3\sum_l \phi_l^4/l^2, \quad (2)$$

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

$$A_1(\phi_{l+1}-2\phi_l+\phi_{l-1})+A_2l^2\phi_l+2NA_3\phi_l^3/l^2=\mu\phi_l. \quad (3)$$

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 ϕ_l for an arbitrary N and μ from the recursion relation Eq. (3). Next, we scale ϕ_l and N with $\epsilon=\Sigma_l\phi_l^2$ as $N'=\epsilon N$ and $\phi_l'=\phi_l/\sqrt{\epsilon}$, respectively. Then we obtain a true solution ϕ_l' for N' and μ. 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-

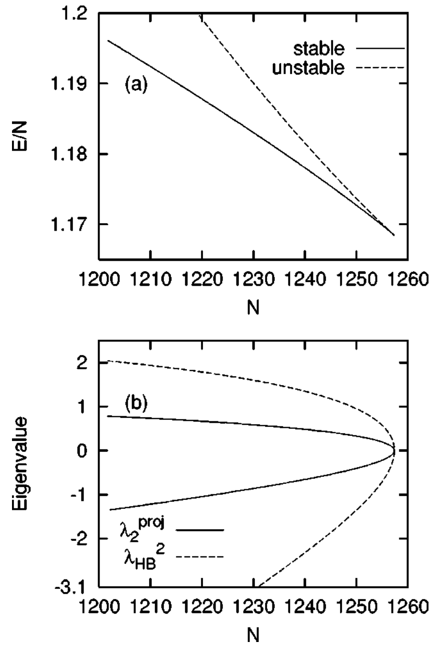

FIG. 1. The energy (a) and the eigenvalue (b) as a function of the bifurcation parameter $x=1-N/N_{cr}$.

ing the fluctuations up to quadratic terms at $\mathbf{\Phi}$, the energy functional E becomes $E=E[\mathbf{\Phi}]+\delta\mathbf{\Phi}\mathbf{H}\delta\mathbf{\Phi}$, where $\mathbf{H}$ is the Hessian matrix whose nonzero elements are $\mathbf{H}_{l,l}=-2A_1+A_2l^2+6NA_3\phi_l^{02}/l^2-\mu$ and $\mathbf{H}_{l,l+1}=\mathbf{H}_{l+1,l}=A_1$. Here, the fluctuations $\delta\mathbf{\Phi}$ cannot be varied independently because they are subject to the normalization constraint. To impose the constraint on the fluctuations, we used the projection matrix $\mathbf{P}$ defined as $\mathbf{I}-\mathbf{\Phi}\otimes\mathbf{\Phi}$, where $\mathbf{I}$ is the identity matrix [13]. Here $\otimes$ means the outer product of two vectors. Substituting $\mathbf{P}\delta\mathbf{\Phi}$ for $\delta\mathbf{\Phi}$, we obtain a projected Hessian as $\mathbf{H}^{proj}=\mathbf{P}^T\mathbf{H}\mathbf{P}$. Each normal mode of $\mathbf{H}^{proj}$ belongs to either of two subspaces. One subspace corresponds to the constraint subspace, and the other one corresponds to the orthogonal subspace whose normal modes are orthogonal to $\mathbf{\Phi}$. Then the stability of the stationary solution is determined by the second lowest eigenvalue λ_2^{proj} of $\mathbf{H}^{proj}$. In Fig. 1(b) we plot λ_2^{proj} and λ_{HB}, which is the lowest frequency of the Hartree-Bogoliubov equation, for both stable and unstable solutions as a function of N. Instability occurs at $N_{cr}=1257.2$, which is identified by a zero value of λ_2^{proj} and λ_{HB}. Beyond the instability point, λ_2^{proj} goes to $-\infty$ implying the collapse of the condensate. Also λ_{HB} becomes 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 λ_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 $\mathbf{\Phi}_0$ and N_{cr}, where $\mathbf{\Phi}_0$ is the solution of the GPE at the bifurcation point N_{cr}, gives

$$
\begin{aligned}
E[\mathbf{\Phi},x]=&E_0[\mathbf{\Phi}_0,0]-xN_{cr}A_3\sum_l\frac{(\phi_l^0)^4}{l^2}\\
&+N_{cr}\Bigg[-x4A_3\sum_l\frac{(\phi_l^0)^3}{l^2}\delta\phi_l+\delta\mathbf{\Phi}'^T\mathbf{H}^{proj}\delta\mathbf{\Phi}'\\
&-x6A_3\sum_l\frac{(\phi_l^0)^2}{l^2}\delta\phi_l^2+(1-x)4A_3\sum_l\frac{(\phi_l^0)}{l^2}\delta\phi_l^3\\
&+(1-x)A_3\sum_l\frac{\delta\phi_l^4}{l^2}\Bigg],
\end{aligned}
\tag{4}
$$

where $\delta\mathbf{\Phi}=\mathbf{P}\delta\mathbf{\Phi}'$, 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 $\delta\mathbf{\Phi}'$ to the constraint subspace. Next, using a linear transformation $\delta\mathbf{\Phi}=\Sigma_{l=2}Q_l\mathbf{e}_{\lambda_l^{proj}}$, where $Q_l=\delta\mathbf{\Phi}\cdot\mathbf{e}_{\lambda_l^{proj}}$, Eq. (4) can be rewritten as a function of Q_l $(l=2,\ldots,L)$,

$$
\begin{aligned}
E[\mathbf{\Phi},x]=&E_0-\alpha x+N_{cr}\Bigg[\sum_{i=3}\lambda_i^{proj}Q_i^2+x\sum_{i=2}K_iQ_i\\
&+x\sum_{ij=2}K_{ij}Q_iQ_j+(1-x)\sum_{ijk=2}K_{ijk}Q_iQ_jQ_k\\
&+(1-x)\sum_{ijkl=2}K_{ijkl}Q_iQ_jQ_kQ_l\Bigg],
\end{aligned}
\tag{5}
$$

where $\alpha=N_{cr}A_3\Sigma_l(\phi_l^0)^4/l^2=-0.802$. The projection of $\delta\mathbf{\Phi}'$ onto the constraint subspace eliminates all terms containing Q_1. Also the term Q_2^2 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,

$$
\begin{aligned}
E[\mathbf{\Phi},x]&=E_0-\alpha x+F_{NM}(Q_2)+F_M[Q_3,\ldots,Q_L]\\
&=E_0-\alpha x+\beta xQ_2+\gamma xQ_2^2+\delta(1-x)Q_2^3\\
&\quad+\eta(1-x)Q_2^4+F_M[Q_3,\ldots,Q_L],
\end{aligned}
\tag{6}
$$

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

$$
\begin{aligned}
F[Q_2]=&E_0-\alpha x+\beta x\kappa^3Q_2+\gamma x\kappa^2Q_2^2\\
&+\delta(1-x)\kappa Q_2^3+\eta(1-x)Q_2^4,
\end{aligned}
\tag{7}
$$

where β, γ, δ, η, and κ are to be determined from the numerical solutions. The parameter κ 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):

$$Q_2^0=\kappa\frac{p}{3}\left[1+2\sqrt{1+B_1t}\cos\left(\frac{1}{3}\tan^{-1}\frac{\sqrt{G(t)}}{1+B_2t}\right)\right]$$
$$=\kappa\frac{p}{3}[1+Z_0],$$

$$Q_2^{\pm}=\kappa\tilde{Q}_2^{\pm}$$
$$=\kappa\frac{p}{3}[1+Z_0/2(-1\pm\sqrt{1-(2p/3Z_0)^3(1+B_2t)})], \tag{8}$$

where $B_1=-3q/p^2$, $B_2=-(27/2p^3)(pq/3+r)$, and $G(t)=(3B_1-2B_2)t+(3B_1^2-B_2^2)t^2+B_1^3t^3$, $t=x/(1-x)$. Notice that Q_2^0 has no physical meaning since it approaches κp as $x\rightarrow 0$, 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^+ and Q_2^- correspond to the stable and unstable branches of Eq. (3), respectively. Let us define $\Delta_Q^{\pm}(x)$ as $(\mathbf{\Phi}_x-\mathbf{\Phi}_0)\cdot\mathbf{e}_{\lambda_2^{proj}}$, where $\mathbf{\Phi}_x$ 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 $\Delta_Q^{\pm}(x)$ for the stable (unstable) branch. Still the value of κ remains to be determined from the scaling of the energy. In Fig. 2(a), we plot $\tilde{Q}_2^{\pm}$ and $\Delta_Q^{\pm}(x)$ for the stable and unstable branches with respect to x, respectively. The $\tilde{Q}_2^{\pm}$ shows good agreements with the numerically obtained $\Delta_Q^{\pm}(x)$ including asymmetric behaviors for a wide range of x (<0.03). The eigenvalues $\lambda^{\pm}$ are obtained by differentiating Eq. (7) twice with respect to Q_2,

$$\lambda^{\pm}=12N_{cr}\xi(1-x)[qt/3-2p/3\tilde{Q}_2^{\pm}+(\tilde{Q}_2^{\pm})^2], \tag{9}$$

where $\xi=\eta\kappa^2$. Here ξ is determined by identifying the numerical values of λ_2^{proj} for the stable branch with λ^+. We confirmed that the same ξ is obtained by identifying λ_2^{proj} of the unstable branch with λ^-. Both λ^+ and λ^- are compared with exact λ_2^{proj} obtained from the branches of stable and unstable solutions, respectively, in Fig. 2(b). Finally, the parameter κ is determined by fitting

$$F[Q_2^+]=E_0-\alpha x+(1-x)\xi\kappa^2[4rt\tilde{Q}_2^++2qt(\tilde{Q}_2^+)^2$$
$$-4p/3(\tilde{Q}_2^+)^3+(\tilde{Q}_2^+)^4]$$

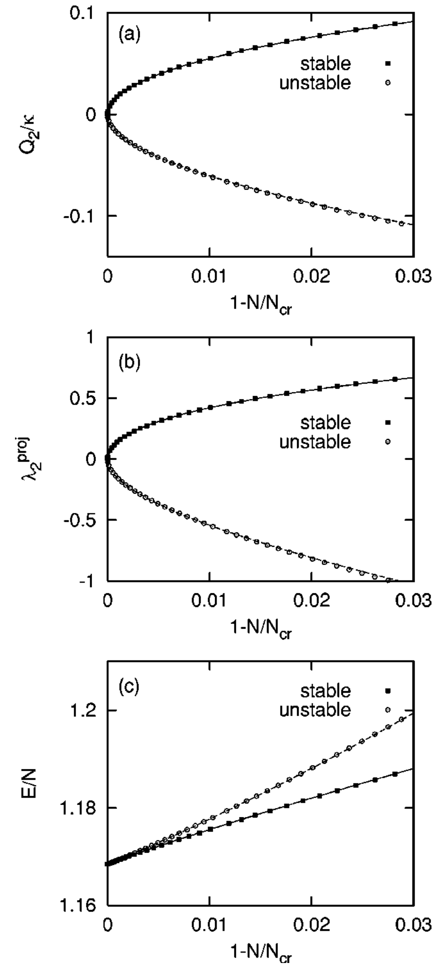

FIG. 2. (a) $\tilde{Q}_2$ as a function of the bifurcation parameter x. The solid and dashed lines correspond to fitted results for the stable and unstable branches, respectively. The filled squares and open circles correspond to a numerical computation for the stable and unstable branches, respectively. (b) The eigenvalue λ_2^{proj} as a function of x. (c) The energy as a function of x.

to E^+ of the stable branch. Figure 2(c) shows the profiles of $F[Q_2^{\pm}]$ 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 vary narrow range of x, our scaling form

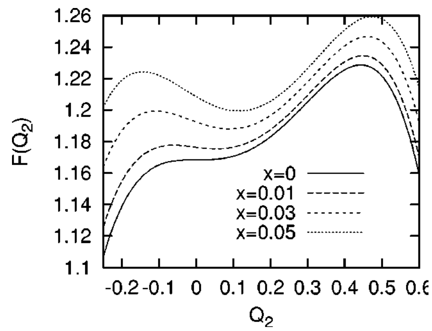

FIG. 3. The catastrophe function F as a function of Q_2 with varying x. At $x=0$, F has a saddle point at $Q_2=0$. For $x>0$, F shows asymmetric behavior around $Q_2=0$ with a local maximum and minimum. The global maximum around $Q_2=0.5$ is an unphysical state.

can be reduced to the same form predicted by the HSN bifurcation, such as $Q_2^{\pm}\sim\pm\sqrt{x}$, $\lambda^{\pm}\sim\pm\sqrt{x}$, and $\Delta E=E^{-}-E^{+}\sim x^{3/2}$ by neglecting quadratic and quartic terms with respect to Q_2 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, $Q_2(y)=y+\Sigma_{n=2}D_n y^n$. By substituting $Q_2(y)$ into Eq. (7) and equating the coefficients of y^n, we have $F[y]=E_0-\alpha x+\eta(1-x)\Sigma_{n=1}F_n(t)y^n$, where

$$F_1=\tilde{\beta},\quad F_2=\tilde{\beta}D_2+\tilde{\gamma},$$

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

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

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

Here, $\tilde{\beta}=\beta\kappa^3/\eta t$, $\tilde{\gamma}=\gamma\kappa^2/\eta t$, and $\tilde{\delta}=\delta\kappa/\eta$. 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 $-1/3\tilde{\delta}$ 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 $D_2=-\tilde{\gamma}/\tilde{\beta}$ 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

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

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

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