Symmetry-breaking thermally induced collapse of dipolar Bose-Einstein condensates

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We investigate a Bose-Einstein condensate with additional long-range dipolar interaction in a cylindrically symmetric trap within a variational framework. Compared to the ground state of this system, little attention has as yet been payed to its unstable excited states. For thermal excitations, however, the latter is of great interest, because it forms the “activated complex” that mediates the collapse of the condensate. For a certain value of the s-wave scattering length our investigations reveal a bifurcation in the transition state, leading to the emergence of two additional and symmetry-breaking excited states. Because these are of lower energy than their symmetric counterpart, we predict the occurrence of a symmetry-breaking thermally induced collapse of dipolar condensates. We show that its occurrence crucially depends on the trap geometry and calculate the thermal decay rates of the system within leading-order transition state theory with the help of a uniform rate formula near the rank-2 saddle which allows the bifurcation to be smoothly passed.

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I. INTRODUCTION

Since the first experimental realization of a Bose-Einstein condensate (BEC) in 1995 [1], the field of ultracold quantum gases has developed rapidly. An important milestone in this development was the condensation of $^{52}$Cr and $^{164}$Dy atoms [2,3], which, due to their large magnetic dipole moments, interact via the anisotropic, long-range dipole-dipole interaction (DDI). Because the latter can be either attractive or repulsive, depending on the orientation of the dipoles, a wealth of new phenomena emerges in these BECs, such as stability diagrams that crucially depend on the trap geometry [4–6], isotropic as well as anisotropic solitons [7–9], biconcave or structured ground state density distributions [10–12], radial and angular rotons [11,13,14], and anisotropic collapse dynamics [15,16]. Investigations of the physics of dipolar systems may in the future be extended with the help of heteronuclear molecules [17–20] or by laser-induced electric dipole-dipole interaction [21].

The stability of a dipolar BEC is in general determined by the interplay of the two-particle interactions present, namely the contact interaction (described by the s-wave scattering length) as well as the DDI, and the geometry and the strength of the trap. In the case of an attractive scattering interaction, the ground state of a harmonically trapped dipolar quantum gas, which we consider in this paper, is metastable and the BEC can decay by a coherent collapse of the condensate. The collapse can be induced by macroscopic quantum tunneling at $T = 0$ [22] or by decreasing the s-wave scattering length into a region where the BEC cannot exist anymore [11].

Another possibility investigated in this paper is the coherent collapse due to thermal excitations of the condensate at finite temperature. We consider temperatures which are, on the one hand, small compared to the critical temperature $T_c$ where the ground state is populated macroscopically so that we have an almost pure condensate. Although modifications will be caused by the interaction of the bosons, a rough estimate of this regime can be obtained from the ideal Bose gas in a harmonic trap for which the fraction $N_0/N$ of condensed particles is given by $N_0/N = 1 - (T/T_c)^3$ [23]. For temperatures $0 < T < T_c$, we then have more than 99% of the bosons in the condensate and can neglect the influence of the thermal cloud. For a $^{52}$Cr condensate that we investigate in the following the critical temperature is $T_c \approx 700$ nK [2]. We therefore consider temperatures of $T < 140$ nK where the thermal excitations are of a collective nature and describe the quasiparticle modes of the whole condensate.

On the other hand, the temperature must be high enough so that collective oscillations of the BEC are activated. As is discussed below, in the relevant region of the scattering length and for experimentally accessible particle numbers, the frequencies of the collective modes can be assigned to a temperature on the order of $T \sim 1$ nK. Thus, in the temperature regime of several tens of nK the latter are sufficiently activated.

Note that, at temperatures higher than those discussed above, a significant number of bosons will occupy excited states so that the Gross-Pitaevskii equation (GPE) will no more be adequate to such a system. In this case the Hartree-Fock-Bogoliubov theory [24,25] can be applied, allowing the investigation of thermally excited BECs at finite temperatures up to the critical temperature. Note further that, at sub-nK temperatures, where collective oscillations are not present anymore, macroscopic quantum tunneling is the dominant decay mechanism. Neither of these temperature regimes is, however, the subject of this paper.

In the temperature regime described above dipolar quantum gases can be well described by a nonlocal GPE, which is usually solved either numerically or by variational approaches. The GPE possesses, apart from the stable ground state, also one or several excited stationary solutions. To date these solutions have received little attention in the literature. However, it is exactly these excited states which form the transition states
harmonic traps in the form can write the extended GPE of dipolar BECs in axisymmetric picture, and discuss the behavior of the potential when one provide the description of the dipolar quantum gas within the rate formula which solves this problem.

The BEC’s thermal decay rate can be obtained by applying transition state theory (TST). However, the standard TST rate formula fails near bifurcations. With the help of a suitable normal form of the potential which describes the entire formula which solves this problem.

The paper is organized as follows: In Sec. II A, we provide the description of the dipolar quantum gas within the variational framework, introduce the equivalent Hamiltonian picture, and discuss the behavior of the potential when one varies the s-wave scattering length. Section II B demonstrates the calculation of the BEC’s decay rate, and in Sec. III we present and discuss the results.

II. THEORY

A. Description of the BEC

Assuming all dipoles to be aligned along the z direction, we can write the extended GPE of dipolar BECs in axisymmetric harmonic traps in the form

\[ i \partial_t \tilde{\psi}(\vec{r},t) = \left( -\Delta + 8\pi \frac{a_{ad}}{a_d} |\tilde{\psi}(\vec{r},t)|^2 + N^4 \gamma \tilde{\rho}^2 + N^4 \gamma_z \tilde{\sigma}_z^2 \right. \]

\[ \left. + \int d^3 \vec{r} \left( 1 - 3 \cos^2 \theta \left| \tilde{\psi}(\vec{r}',t) \right|^2 \right) \tilde{\psi}(\vec{r},t) \right). \]

(1)

Here, \( \tilde{\psi}(\vec{r},t) \) is the scaled condensate wave function, \( \gamma \), \( \gamma_z \) are the dimensionless trap frequencies in radial and z directions, \( a/a_d \) denotes the scaled s-wave scattering length, and \( \theta \) is the angle between the z axis and the vector \( \vec{r} - \vec{r}' \). We use “natural units” [26] for the length \( a_d = m \mu / (2\pi) \), energy \( E_d = \hbar^2 / (2m a_d^2) \), and frequency \( \omega_d = E_d / \hbar \), which are defined using the mass of the bosons, their magnetic moment \( \mu \), and the vacuum permeability \( \mu_0 \). Furthermore, we apply the particle number scaling \( N = \tilde{N} \tilde{\rho} \), \( \tilde{\rho} = N^{-3/2} \tilde{\psi} \), \( E = \tilde{E} \), \( \tilde{\rho} = N^{-1} \tilde{\psi} \), and \( \omega = N^{-1} \omega_d \) in order to eliminate the explicit occurrence of the particle number \( N \) in the interaction terms in Eq. (1). Also, in what follows the inverse temperature is measured by the dimensionless quantity \( \beta = E_d / k_B T \).

Since the unstable excited eigenstates of Eq. (1) are not accessible via imaginary time evolution on a grid, we resort to a variational approach. Because the bosons are trapped harmonically a natural choice is a Gaussian trial wave function [27–34]

\[ \tilde{\psi}(\vec{r},t) = N \prod_{\sigma=x,y,z} \exp \left( -\frac{\sigma^2}{8q_\sigma^2} + ip_\sigma \sigma^2 \frac{4q_\sigma}{4q_\sigma} \right), \]

(2)

which well approximates the true wave function as long as the interactions between the bosons are not too strong. Here \( N \) is the normalization factor of the wave function, \( \int d^3 \vec{r} |\tilde{\psi}(\vec{r},t)|^2 = 1 \), and \( q_\sigma \) and \( p_\sigma \) are time-dependent variational functions. Note that the Cartesian geometry of the ansatz is capable of describing \( m = 0 \) (breathing mode) and \( m = 2 \) (quadrupole mode) collective oscillations of the condensate and therefore covers the two most important modes of the system.

Even though it is well known that the simple ansatz (2) with a single Gaussian will only yield qualitative results, it is crucial because it is the only access to dipolar BECs that can globally be mapped to an equivalent Hamiltonian system, \( H = \vec{p}^2 / 2 + V(\vec{q}) \) [35]. The existence of a Hamiltonian, however, is essential for the application of TST and the derivation of the subsequent rate formula near a rank-2 saddle, since both are formulated in phase space. As shown in Ref. [35] the potential \( V(\vec{q}) \) reads

\[ V(\vec{q}) = \frac{1}{8q_x} + \frac{1}{8q_y} + \frac{1}{8q_z} + \left| \frac{z}{\sqrt{8q_x q_y q_z}} \right| a_{ad} + 2N^4 \gamma^2_\rho (q_x^2 + q_y^2) + 2N^4 \gamma^2_z \]

\[ + \frac{1}{24\sqrt{2}\pi q_z} \left[ \frac{1}{q_z^2} \mathcal{R}_D \left( \frac{q_x^2}{q_z^2}, \frac{q_y^2}{q_z^2}, 1 \right) - \frac{1}{q_y q_z} \right], \]

(3)

where \( \mathcal{R}_D(x,y,z) = \frac{1}{2\pi} \int_{-\infty}^{\infty} (x + t)(y + t)(z + t)^{-1/2} dt \) is an elliptic integral in Carlson form [36]. For given physical values of the scattering length and the trap frequencies the potential fully describes the dynamics of the BEC in the Hilbert subspace of the variational ansatz (2). In what follows we fix the values of the mean trap frequency to \( N^2 (\gamma^2_\rho \gamma^2_z)^{1/3} = 3.4 \times 10^4 \) and of the trap aspect ratio to \( \lambda = \gamma_z / \gamma_\rho = 50 \), if not stated otherwise, and vary \( a_{ad} \).

Note that, because of the large aspect ratio of the trap, the dipoles are predominantly aligned in side-by-side configuration where they repel each other and stabilize the BEC against collapse. In the following, we, therefore, only consider the regime of a negative s-wave scattering length \( a/a_d < 0 \) which counteracts this effect.

Figure 1 shows contour plots of the potential (3) for several values of the scattering length \( a/a_d \) and fixed coordinate \( q_z \). Below a critical value, \( a_{ad} < a_{crit} \) [Fig. 1(a)], there exists no stationary point of the potential. Two of these emerge in a tangent bifurcation at \( a_{crit} \approx -0.227 \), and both are cylindrically symmetric. One represents the stable ground state of the BEC, and the other is an unstable excited state [Fig. 1(b)]. At the scattering length \( a_{ab} \approx -0.226 \) two additional and nonaxisymmetric states emerge from the central saddle in a pitchfork bifurcation, forming two satellite saddles [Figs. 1(c) and 1(d)] and turning the central one into a rank-2 saddle.

The potential (3) allows for a direct interpretation in terms of reaction dynamics of thermally excited dipolar condensates: In the case \( a_{crit} < a/a_d < a_{crit} \), i.e., in the region where only the center saddle exists [Fig. 1(b)], a sufficient thermal excitation of the BEC may allow the system to cross the center saddle and to escape to \( q_x, q_y \rightarrow 0 \), which means the collapse of the BEC. In this case the reaction path will always be located on the angle bisector, and thus this represents a condensate which
with an area of lower energy than the central one the reaction path will probably lie on a saddle, respectively, and $V_0^{\perp}$ is the energy difference between the TS and the ground state.

In the cases $a/a_d \ll a_{pb}$ and $a/a_d \gg a_{pb}$, i.e., far away from the bifurcation, Eq. (5) yields an appropriate approximation for the reaction rate, since then the reaction will either proceed over the central saddle or proceed over one of the satellites. (In the latter case, the rate (5) must be doubled because there are two saddles.) However, in the vicinity of the bifurcation ($a/a_d \approx a_{pb}$), Eq. (5) will fail: Mathematically this is because one of the frequencies $\omega_{i}^{(0)}$ occurring in the denominator will vanish at the bifurcation, leading to the divergence of the reaction rate. Physically speaking, it will fail because the center and satellite saddles are separated by energies of $k_B T$ or less, and reactive trajectories can pass over the central saddle with nearly the same probability as over the satellites.

Since close to the bifurcation the quadratic expansion of the potential is obviously not adequate to reproduce the correct behavior, we need a more accurate approximation. It is provided by the classifications of catastrophe theory [38,39], and we therefore apply a change of coordinates $q' \rightarrow x$ that maps the potential $V(q', q_i = 0)$ to a suitable normal form $V_0 + U(x)$. The remaining integral in Eq. (4) then has the form

$$I = \int d^2x \phi(x) e^{-\beta U(x)},$$

where $\phi(x)$ is the Jacobi determinant arising from the transformation, and the reaction rate reads

$$\tilde{\Gamma} = \frac{\Omega^{(0)}}{2\pi} e^{-\beta V_0^\perp} I.$$  

A suitable normal form describing the bifurcation of the transition state in the axisymmetric trap is

$$U(x) = \frac{1}{4} x_2^2 + \frac{u}{2} x_2^2 + \frac{1}{2} \sum_{i=3}^d \left( \omega_i^{(0)} \right)^2 x_i^2.$$  

It is quadratic in all variables but one. The number and type of stationary points of $U$ depend on the value of the parameter $u$. By a suitable choice of $u$, we reproduce the bifurcation of saddle points that is found in the physical potential $V$.

For $x_i = 0$ ($i \neq 2$) and $u < 0$ the function $U(x)$ has a maximum at $x_{2,ss} = 0$ (center saddle) and two minima at $x_{2,ss} = \pm \sqrt{-u}$ (satellite saddles) with $U(x_{2,ss}) = -u^2/4$. In the case $u > 0$, $x_{2,ss} = 0$ is a minimum and the other stationary points $x_{2,ss}$ are imaginary. With the energy difference $\Delta V^\perp$ between the central saddle and the satellite saddles we further define the unfolding parameter $u = \pm 2\sqrt{\Delta V^\perp}$ and choose it to be negative if all stationary states are real and to be positive otherwise. With this choice Eq. (8) by construction reproduces the physical energy gap of the saddle configuration over the whole range of the scattering length $a/a_d$.

What remains is to determine the prefactor $\phi(x)$ in Eq. (6) in such a way that the flux integral reproduces the standard TST rate far away from the bifurcation. In the case $u \rightarrow \infty$ (only the center saddle) we can return to the quadratic approximation of the potential, and because the prefactor varies slowly we can...
regard it as constant. In this limit we have

\[ I \approx \sqrt{\frac{2\pi}{\beta u}} \phi(0) \equiv \frac{1}{\Omega_{cs}^{\beta u}}, \quad (9) \]

where "≡" denotes the requirement that the conventional TST result is to be reproduced. Analogously in the limit \( u \to -\infty \) we require

\[ I \approx 2 \times \phi(x_\infty) \sqrt{\frac{\pi}{-\beta u}} e^{-\beta u x_\infty^2/4} \equiv 2 \times \frac{1}{\Omega_{cs}^{(b)}}, \quad (10) \]

to reproduce the flux over the two satellite saddles. Since \( \phi(x) \) must be an even function, we finally write the following as its lowest-order Taylor expansion,

\[ \phi(x) = \phi(0) - \frac{\phi(x_\infty) - \phi(0)}{u} x_\infty^2, \quad (11) \]

and, once the values of \( \phi(0) \) and \( \phi(x_\infty) \) have been determined from Eqs. (9) and (10), we solve the remaining integral in Eq. (7) numerically.

In a different setting, the corrections to TST rates that are due to rank-2 saddles were recently estimated by Marsson et al. [40], who calculated the energy ridge that connects the rank-1 saddle to the rank-2 saddles. In contrast to ours, their method takes account of the precise shape of the potential along the ridge. The present approach provides a rate formula that applies on both sides of, and arbitrarily close to, the bifurcation. It also offers the advantage of greater simplicity because it only requires information about the saddle points themselves. Via the frequencies \( \omega_0^{(b)}, \omega_1^{(b)} \), the influence of degrees of freedom transverse to the ridge is taken into account.

III. RESULTS

Figure 2 shows the thermal decay rates of the dipolar BEC in leading-order TST calculated from Eq. (5) in comparison with the results obtained from the uniform rate formula for the rank-2–rank-1 saddle configuration, Eq. (7). The first case solely considers the energetically lowest saddle(s) (lines) while the second case takes into account the complete configuration of saddles (dots). In the calculations using the conventional TST rate formula (lines), the divergence of the decay rate at \( a/a_d \approx -0.22657 \) is obvious. By contrast, the uniform solution (dots) passes the bifurcation smoothly. We again emphasize that the collapse of the BEC will be cylindrically symmetric on one side of the bifurcation and symmetry-breaking on the other side. Near the bifurcation, however, a clear distinction can no longer be made.

In the calculation the particle number scaled temperatures have been adapted to a \( ^{52}\text{Cr} \) BEC with a magnetic moment of \( \mu = 6 \mu_B \) (\( \mu_B \) is the Bohr magneton) and a particle number of \( N = 50,000 \) as it has been realized experimentally by Griesmaier et al. [2]. For this number of bosons the values \( \beta = 0.03 \) to \( \beta = 0.06 \) correspond to temperatures between \( T = 65 \text{nK} \) and \( T = 130 \text{nK} \) which are clearly below the critical temperature of \( T_c \approx 700 \text{nK} \) so that the treatment within the Gross-Pitaevskii framework is justified.

Note that, on the other hand, these temperatures are high enough to activate collective oscillations of the BEC: In the relevant region of the scattering length, the frequencies of the monopole mode and the quadrupole mode are, both, on the order of \( \omega \sim 10,000 \). For the above-mentioned particle number, this means an oscillation frequency of \( \omega \approx 107 \text{s}^{-1} \). Assigning to this frequency an energy of \( E \sim h\omega \) as well as the temperature \( T \sim E/k_B \), we find a value of \( T = 0.8 \text{nK} \) to determine the order on which collective oscillations are activated. Thus, for the temperatures given above the latter are sufficiently present.

For experiments it will be of great interest in which region of the physical parameters (trap frequency and scattering length) a symmetry-breaking collapse is to be expected. Figure 3 shows that the existence of the symmetry-breaking states and the corresponding regions of the scattering length crucially depend on the trap aspect ratio. While for small \( \lambda \lesssim 2.8 \) (including prolately trapped condensates \( \lambda < 1 \), not shown) only the cylindrically symmetric excited states exist, the additional symmetry-breaking states appear for oblate

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**FIG. 2.** (Color online) Scaled decay rate \( \tilde{\Gamma} = N^2 \Gamma \) of the dipolar BEC in dependence of the scattering length \( a/a_d \) and for different temperatures \( \beta = N^{-1} \beta \). The lines show the results calculated from the conventional TST rate formula (5) and the dots show the corresponding reaction rate obtained from the uniform rate formula (7). The temperatures \( T \) as well as the decay rate \( \Gamma \) have been calculated for \( ^{52}\text{Cr} \) BECs with a particle number of \( N = 50,000 \).

**FIG. 3.** (Color online) Stability diagram of the unstable excited state(s) of the GPE in dependence of the scattering length \( a/a_d \) and the trap aspect ratio \( \lambda \). There exists no excited state, only the symmetric state, or, in addition, two symmetry-breaking states.
condensates with $\lambda \gtrsim 2.8$. The more oblate the BEC the larger becomes the region in which these states are present. In contrast, increasing the trap aspect ratio, the parameter region of the scattering length with $a_{\text{cen}} < a < a_{\text{ph}}$ becomes smaller and vanishes for $\lambda \to \infty$. We therefore expect the trap aspect ratio to be the decisive tool to switch between the two scenarios in an experiment. Note that the curve in Fig. 3 for the critical scattering length of course corresponds to the one published by Koch et al. [4].

IV. CONCLUSION AND OUTLOOK

We have investigated a thermally excited dipolar BEC in a cylindrically symmetric trap. Within a variational framework we observed that the unstable excited state of the system which forms the “activated complex” on the way to the collapse of the condensate undergoes a bifurcation. This divides the parameter region of the $s$-wave scattering length into a region with cylindrically symmetrical collapse and one where the collapse occurs with broken symmetry. With the help of a uniform rate formula, we were able to calculate the corresponding reaction rate over the whole range of the scattering length within leading-order TST and to smoothly pass the bifurcation. Moreover, the occurrence of the additional bifurcation strongly depends on the trap geometry which allows one to switch between the two scenarios in experiments.

In order to improve the results quantitatively, the procedure described here can be extended to coupled Gaussian wave functions, whose power to reproduce or even to exceed the quality of numerical results has already been proven [41,42]. We have shown elsewhere [43,44] that it is possible to construct a Hamiltonian also for the case of coupled Gaussians which then allows for the application of TST. While in the case of a long-range $1/r$-interaction we could show that converged results for the decay rate are only shifted to higher values of the scattering length, the situation is different in dipolar BECs: The bifurcation of the TS leading to the symmetry-breaking stationary states also exists in the case of coupled wave functions; however, in the latter case even more bifurcations occur when the number of Gaussians is increased. The even richer thermal collapse scenarios and decay rates of dipolar BECs described by coupled Gaussians are a challenge for currently ongoing research.

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