MEAN-FIELD MODELING OF COLLAPSE ONSET IN A DIPOLAR BOSE–EINSTEIN CONDENSATE USING GPELAB

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Abstract. We present a mean-field numerical study of the stability boundary of a two-dimensional dipolar Bose–Einstein condensate (BEC), computed with the GPELab MATLAB toolbox. Ground states of the Gross–Pitaevskii equation (GPE) are obtained by imaginary-time propagation while the dipolar interaction strength is increased step by step. Stable condensates with a central density maximum are found at weak dipolar coupling; a density dip and then a ring-shaped profile develop as the coupling grows, and the iteration ceases to converge between dipolar strengths of 1.63 and 1.65 (in the units of the solver's built-in dipolar example). Beyond this point the imaginary-time energy diverges, indicating that no stable stationary state exists within this model. The results are a characterization of mean-field behavior only and are preliminary with respect to numerical convergence studies.

Keywords: Bose–Einstein condensate; Gross–Pitaevskii equation; dipolar interaction; collapse; GPELab; imaginary-time propagation

1. Introduction: subject and relevance

Subject. A dilute BEC at zero temperature is described, in the mean-field approximation, by the Gross–Pitaevskii equation, a nonlinear Schrödinger equation for the condensate wave function $\psi(r, t)$:

$$i\frac{\partial\psi}{\partial t} = [\, -\frac{1}{2}\nabla^2 + V(r) + \beta|\psi|^2 + \lambda\,(U_{dd} * |\psi|^2)\,]\,\psi,$$

where V is the trapping potential, β is the strength of the short-range contact interaction, U_dd is the long-range, anisotropic dipole–dipole potential, λ is the dipolar strength and ∗ denotes convolution. When the net interaction is attractive, or when the dipolar term dominates the contact term, the condensate can become unstable and collapse: its density grows locally until the mean-field description ceases to be valid. Collapse of attractive condensates was observed in ^{7}Li and ^{85}Rb [1, 2], and in dipolar gases of chromium, dysprosium and erbium it is controlled by the competition between contact and dipolar interactions [3–6].

Relevance. Strongly dipolar gases are now a main platform for studying quantum droplets, supersolidity and roton-type instabilities [7–9]. In all of these phenomena the mean-field stability boundary is the reference point: it marks where purely mean-field theory fails and beyond-mean-field corrections, such as the Lee–Huang–Yang term, become decisive [7]. A reproducible, openly available numerical procedure for locating this boundary is therefore useful both for theory and for planning experiments. GPELab provides such a platform for stationary states and dynamics [10, 11] , but systematic, documented stability scans with it for dipolar condensates are less common in the literature.

2. Research objective

The objective is to characterize, within the mean-field GPE, how the ground state of a two-dimensional dipolar BEC changes with increasing dipolar interaction strength, and to bracket the

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strength at which a stable stationary state ceases to exist. Specific goals are: (i) to follow the evolution of the density profile and energy along a one-parameter sequence of runs; (ii) to determine the interval in which imaginary-time propagation changes from convergent to non-convergent; and (iii) to document the procedure so that it can be repeated and extended to dynamical collapse simulations.

3. Methods

All calculations used GPELab (Antoine and Duboscq) [10, 11], a MATLAB toolbox for stationary and time-dependent GPEs, in a two-dimensional configuration with a dipolar nonlinearity and the contact strength $\beta = 100$ of the toolbox's dipolar example. The model was run without modification of the example script apart from the dipolar strength parameter (RhoDipole), which was varied one value at a time.

Ground states. Stationary states were computed by imaginary-time propagation, i.e. a normalized gradient flow that decreases the energy at fixed norm [12, 13]. The time step is advanced with a Strang-type split-step Fourier scheme, in which kinetic and potential terms are treated in alternating sub-steps [11, 13]. The dipolar potential is evaluated as a convolution through fast Fourier transforms [13]. Iteration stops when the change between successive iterates falls below the solver's stopping criterion.

Resolution. The spatial grid should resolve the healing length of the condensate; spatial step and domain size must be chosen relative to this length so that the density structure, particularly the ring-shaped profile, is not an artifact of the discretization.

Parameter continuation. The dipolar strength was increased through the values 0.5, 1.2, 1.5, 1.6, 1.63, 1.65, 1.7, 1.8 and 2.0. For each run we recorded the convergence status, the density profile, the peak density and the energy. The collapse threshold is bracketed by the last convergent and first non-convergent values.

Dynamics (planned). Real-time propagation with the same split-step scheme [11] will be used to follow the collapse itself after the threshold is bracketed.

4. Main results

The sequence of runs gave three regimes (Table 1).

Dipolar strength	Outcome
0.5, 1.2	Converged; blob-like density with a central maximum
1.5	Converged; a central density dip begins to form
1.6	Converged; ring-shaped density, peak density 0.0658, energy 4.23
1.63	Marginal; stopping criterion 1.6×10^{-4} reached at iteration 1425 without full convergence; square-like ring
1.65	Iteration failed
1.7, 1.8, 2.0	Diverged; energies in the hundreds to thousands

Table 1. Outcome of imaginary-time ground-state calculations versus dipolar strength.

First, at weak coupling the ground state is a smooth, centrally peaked profile. Second, as the dipolar strength approaches 1.5–1.6 the central density is depleted and a ring forms, a change of shape that is qualitatively consistent with the density-redistribution and biconcave profiles known for dipolar

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condensates in oblate geometries [3, 14]. Third, near 1.63 the iteration converges only marginally and the profile becomes square-like, which is typical of a state approaching an instability, and from 1.65 upwards the energy no longer settles. In this model, the stability boundary therefore lies between 1.6 (clearly converged) and 1.65 (failed), with 1.63 marginal.

Two cautions apply. The failure of imaginary-time propagation shows that no stable stationary state was found by this procedure; it is an indicator of the onset of collapse, not a measurement of collapse dynamics. And the bracket rests on single runs of one example configuration: sensitivity to grid spacing, time step and tolerance has not yet been tested, so the marginal point near 1.63 may partly reflect slow convergence rather than a sharp threshold.

5. Scientific and practical significance

Scientific. The work supplies a transparent mean-field baseline for the stability boundary of a dipolar condensate, together with a continuation protocol that separates convergent, marginal and divergent cases. Because mean-field theory omits quantum fluctuations, the bracketed boundary also identifies where beyond-mean-field effects must be included to describe stabilized states such as quantum droplets [7, 8]. The honest scope of the study is a characterization of the mean-field model, not a prediction for a specific experimental species.

Practical. The procedure uses an open, documented toolbox and can be repeated by other groups, which makes it suitable as a benchmark and as a teaching and training example for graduate students. After rescaling to physical units, such scans can guide the choice of trap geometry and interaction strength in experiments with Cr, Dy and Er [4–6, 15]. Next steps are a grid and time-step convergence study, a physical-unit mapping, and real-time collapse simulations.

References

1. C. C. Bradley, C. A. Sackett, R. G. Hulet, Bose–Einstein condensation of lithium: observation of limited condensate number, Phys. Rev. Lett. (1997).
2. E. A. Donley et al., Dynamics of collapsing and exploding Bose–Einstein condensates, Nature (2001).
3. T. Lahaye, C. Menotti, L. Santos, M. Lewenstein, T. Pfau, The physics of dipolar bosonic quantum gases, Rep. Prog. Phys. (2009).
4. A. Griesmaier, J. Werner, S. Hensler, J. Stuhler, T. Pfau, Bose–Einstein condensation of chromium, Phys. Rev. Lett. (2005).
5. M. Lu, N. Q. Burdick, S. H. Youn, B. L. Lev, Strongly dipolar Bose–Einstein condensate of dysprosium, Phys. Rev. Lett. (2011).
6. K. Aikawa et al., Bose–Einstein condensation of erbium, Phys. Rev. Lett. (2012).
7. I. Ferrier-Barbut, H. Kadau, M. Schmitt, M. Wenzel, T. Pfau, Observation of quantum droplets in a strongly dipolar Bose gas, Phys. Rev. Lett. (2016).
8. L. Chomaz et al., Quantum-fluctuation-driven crystallization transition in a dipolar Bose–Einstein condensate, Phys. Rev. X 6, 041039 (2016).
9. H. Kadau et al., Observing the Rosensweig instability of a quantum ferrofluid, Nature (2016).
10. X. Antoine, R. Duboscq, GPELab, a Matlab toolbox to solve Gross–Pitaevskii equations I: computation of stationary solutions, Comput. Phys. Commun. (2014).
11. X. Antoine, R. Duboscq, GPELab, a Matlab toolbox to solve Gross–Pitaevskii equations II: dynamics and stochastic simulations, Comput. Phys. Commun. (2015).

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12. W. Bao, Q. Du, Computing the ground state solution of Bose–Einstein condensates by a normalized gradient flow, SIAM J. Sci. Comput. (2004).
13. W. Bao, Y. Cai, H. Wang, Efficient numerical methods for computing ground states and dynamics of dipolar Bose–Einstein condensates, J. Comput. Phys. (2010).
14. S. Ronen, D. C. E. Bortolotti, J. L. Bohn, Bogoliubov modes of a dipolar condensate in a cylindrical trap, Phys. Rev. A (2006).
15. F. Dalfovo, S. Giorgini, L. P. Pitaevskii, S. Stringari, Theory of Bose–Einstein condensation in trapped gases, Rev. Mod. Phys. (1999).

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